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(71) Applicant (for all designated States except US): KARO BIO AB [SE/SE]; Novum, S-141 57 Huddinge (SE).

(72) Inventors; and

(75) Inventors/Applicants (for US only): ÖHMAN, Lars [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). BONN, Tomas [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). CARLQUIST, Mats [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). ENGSTRÖM, Owe [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). GOEDE, Patrick [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). HEDFORS, Asa [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). HOLMGREN, Erik [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). KOEHLER, Konrad [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). BZOZOWSKI, Andrzeji, Marek [GB/GB]; The University of York, Heslington, York YO1 5DD (GB). PIKE, Ashley, Charles, William [GB/GB]; The University of York, Heslington, York YO1 5DD (GB). HUBBARD, Roderick, Eliot [GB/GB]; The University of York, Heslington, York YO1 5DD (GB).

(74) Agent: WITHERS & ROGERS; 4 Dycr's Buildings, Holborn, London ECIN 2JT (GB).

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#### (54) Title: ESTROGEN RECEPTOR LIGANDS

#### (57) Abstract

Crystal comprising at least part of the ERa ligand binding domain, optionally bound to a ligand, ligands that bind to ER receptors, and methods of designing them, and a homology model of the  $ER\beta$  receptor.

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#### **Estrogen Receptor Ligands**

This invention relates to estrogen receptor ligands. More particularly, the present invention relates to ligands which will bind to estrogen receptors, crystals of such receptors, including crystals of receptor and ligand, synthetic ligands, methods of using such synthetic ligands and methods for designing ligands which will bind to the estrogen receptor.

The thyroid hormone receptor (TR) is known and its three-dimensional structure, and hence its ligand binding domain, has been determined. Knowledge of the three-dimensional structure has enabled a better understanding of the modes of ligand binding and the determination of the optimum conformation of ligand to bind to the receptor. This understanding will provide a pharmacophore model usable in the design of ligands, such as drugs, to bind to the thyroid receptor. It is generally believed in the art that the TR structure also provides a guide to the design of ER ligands.

Estrogen steroid hormone and thus the estrogen receptor (ER) is a member of the steroid hormone receptor family. Its primary natural ligand is estradiol (E2). However, it is known that a large number of structurally diverse non-steroidal compounds such as raloxifene, centchroman, coumestrol, diethylstilbesterol, esculin, tamoxifen, zearalenone, and zindoxifen also bind to the estrogen receptor (Fig. 8). The majority of these non-steroidal estrogen receptor ligands contain 2-4 carboxyclic, aromatic, and/or heterocyclic rings connected by a 1-3 atom chain. One or more of the rings may be fused with the central atom chain or with each other.

It has been proposed that the receptor possesses a multi-functional modular structure potentially having discrete domains for DNA binding, ligand binding, and transactivation. The ligand binding domain (LDB) has been designated domain E and is the largest domain of the estrogen receptor. The ligand binding domain includes a ligand recognition site and regions for receptor dimerzation, interaction with heat

shock proteins, nuclear localization and ligand dependent transactivation.

A review of the structure and functioning of the estrogen receptor is provided in an article by Katzenellenbogen, J. et al., Steroids, (1997) 62(3): 268-303.

It is known that compounds which bind to the estrogen receptor are potentially useful in the treatment a wide range of disease states. These include estrogen agonists for treatment of disease linked to estrogen deficiency (e.g., osteoporosis, cardiovascular and neurodegenerative diseases in post menopausal women) and estrogen antagonists for treatment of breast and uterine cancer. Furthermore, it is known that certain ligands such as tamoxifen display mixed agonist/antagonist action (that is they are either estrogen agonists, estrogen antagonists, or a partial estrogen antagonists when binding to the estrogen receptors of different tissues) and such compounds may simultaneously prevent bone loss and reduce the risk of breast cancer. It is further known that benzothiophenes are usable as agonists or antagonists to steroid hormones, and that it is possible to modify their binding mechanics, for example the binding affinity, by changing the substituent groups at various positions on the molecule. Therefore, it would be desirable to be able to design ligands which are recognizable by and able to bind to the estrogen receptor. Additionally, it would be desirable to know the three dimensional structure of the estrogen receptor. Such knowledge would be useful for the design of compounds intended to bind to the estrogen receptor. The present inventors have been able to produce an estrogen receptor crystal and to determine from that the three dimensional structure of the estrogen receptor. Unexpectedly, the thus determined ER structure reveals that the TR structure does not provide a good model for binding of ligands to ER.

Therefore, in a first aspect the present invention provides an estrogen receptor ligand binding domain crystal.

In a second aspect, the present invention provides ligands, particularly synthetic ligands, of estrogen receptors by use of the crystals.

In a third aspect of the invention, methods for designing ligands which will bind to the estrogen receptor are provided. Such methods use three dimensional models based on the crystals of the estrogen receptor. Generally, such methods comprise, determining compounds which are likely to bind to the receptor based on their three dimensional shape compared to that of the estrogen receptor and in particular the ligand binding domain of the estrogen receptor. Preferably, those compounds have a structure which is complementary to that of the estrogen receptor. Such methods comprise the steps of determining which amino acid or amino acids of the ligand binding domain of the estrogen receptor interacts with the binding ligand, and selecting compounds or modifying existing compounds, to improve the interaction. Preferably, improvements in the interaction are manifested as increases in the binding affinity but may also include increases receptor selectivity and/or modulation of efficacy.

Preferably, the ligands bind to the ER with a high binding affinity, for example within the range of 20-2000 pmol.

The ligands may bind tightly bind to the ER yet not up-regulate gene expression thereby inhibiting the action of estradiol and estradiol mimetics. Thus, the invention also provides a method of inhibiting the activity of estradiol or estradiol mimetics by providing ligands which bind to ER with a high affinity, blocking the activity of estrogens. Alternatively, binding of the ligand to the ER may cause conformational changes to the ER inhibiting further binding thereto. The invention further provides a method of inhibit estradiol activity in an animal, the method comprising administering to the animal a ligand which binds to at least the LBD, of the ER with high affinity and blocks binding of further ligands to at least the LDB of the ER. Such ligands are useful in, for example, the treatment of estrogen receptor mediated diseases in females.

## Structure Based Design of ER Ligands

The present work has elucidated the structure of the ligand binding cavity of

the estrogen receptor. Knowledge of the structure of this cavity has utility in the design of structurally novel ER ligands and in the design of non-obvious analogs of known ER ligands with improved properties. These enhanced properties include one or more of the following: (1) higher affinity, (2) improved selectivity for either the α-or β-isoform of the ER, and/or (3) a designed degree of efficacy (agonism vs. partial agonism vs. antagonism). Without knowledge of the ER structure, modifications to produce ligands with enhanced properties and a reasonable likelihood of success would not be available to those skilled in the art. The ER receptor structure also has utility in the discovery of new, structurally novel classes of ER ligands. Electronic screening of large, structurally diverse compound libraries such as the Available Chemical Directory (ACD) will identify new structural classes of ER ligands which will bind to the 3-dimensional structure of the estrogen receptor. Additionally the ER structure allows for "reverse-engineering" or "de novo design" of compounds to bind to the ER.

### (1) Enhanced Affinity

The present work has revealed the presence of receptor defined  $\beta$ - and  $\alpha$ -face cavities centered respectively above and below the B- and C-rings of estradiol.

The present invention provides new ligands which exploit this discovery by filling the  $\alpha$ - and  $\beta$ -face cavities.

Preferably, the ligand fills at least one of the  $\alpha$ - and  $\beta$ -face cavities so as to exclude water from the cavity or cavities.

The ligands produced in accordance with the invention bind more effectively to the ER than estradiol. The ligand may bind with twice the binding affinity of estradiol, preferably three times the affinity, and most preferably ten or more times the affinity.

Modifications to the steroid nucleus may be made at the positions marked in R in Fig. 8a and 8b ( $\alpha$ -substitution at the 7-, 9-, 12-, 14-, 16-, and 17-positions;  $\beta$ -substitution at the 8-, 11-, 15-, and 18-positions). Preferably, those substituents are hydrophobic substituents, e.g., methyl, ethyl, iso-propyl, chlorine, bromine, or iodine.

Modifications to 2-aryl benzothiophenes may be made at the 2'-, 3'-, and 6'-positions (Fig. 8c) in order to fill the  $\alpha$ - and  $\beta$ -face cavities of ER. Preferably substituents should be present in at least two of the following three positions: 3, 2', or 6' so that a perpendicular conformation between the B- and C-rings of the 2-aryl benzothiophene nucleus is enforced. This perpendicular conformation facilitates the positioning of the 2'-, 3'-, and 6'-substituents in the  $\alpha$ - and  $\beta$ -face cavities of ER.

In a manner analogous to the benzothiophene series, the affinity of other classes of non-steroidal ER ligands may be enhanced by substitution of small hydrophobic substituents at positions marked R2', R3', and/or R6' in Fig. 8C.

Preferably, the ligand produce in accordance with the invention fills at least one of the  $\alpha$ - and  $\beta$ -cavities of the ER without perturbing the remainder of the ER structure.

Another aspect of this invention reveals an unfilled hydrophobic cavity in the raloxifene/ER complex. Filling this cavity with hydrophobic substituents so as to exclude water will enhance binding affinity. This cavity may be filled by positioning a hydrophobic substituent on the ethoxyphenyl sidechain  $\alpha$  to the piperidinyl nitrogen atom of raloxifene. This hydrophobic substituent may be a linear alkyl or perfluoroalkyl group (-CH<sub>3</sub> to -C<sub>10</sub>H<sub>21</sub>, -CF<sub>3</sub> to -C<sub>10</sub>F<sub>21</sub>), benzyl (-CH<sub>2</sub>Ph, or methylene cyclohexyl (-CH<sub>2</sub>C<sub>6</sub>H<sub>11</sub>).

In a third aspect of this invention, examination of the ER structure reveals that the hydroxyl group at position-3 of estradiol or position-6 of raloxifene form hydrogen bonding interactions with Glu-353 and Arg-394 (Fig. 5a and 5b). It is known that

replacement of the hydroxyl group at position-3 of estradiol or position-6 of raloxifene results in a decrease in affinity for the ER. The invention reveals the reason for this reduction in affinity: while one of the hydrogen atoms of the amino group forms a favorable hydrogen bonding interaction with Glu-353, the second hydrogen atom forms an unfavorable electrostatic interaction with Arg-394. Furthermore this invention reveals a method for enhancing the affinity of 3-amino analogs of estradiol and 6-amino analogs of raloxifene: replacement of one of the two hydrogen atoms of the amino group with an alkyl group to produce a secondary amino group. Alternatively, the amino group may be replaced with a guanidino group (Fig. 8e) which will pick up two additional hydrogen bonding interactions, the first is a salt bridge to Glu-353 and the second is a hydrogen bonding interaction with a backbone carbonyl group in residue Leu-387. Similar enhancement of affinity for the ER may be achieved by replacement of the guanidino group with a fused 2-aminopyrrole (Fig. 8e).

In a closely related aspect of this invention, an understanding is provided for the reduction in affinity for the ER seen in ether derivatives at either position-3 of estradiol or position-6 of raloxifene: electrostatic repulsion between the ether oxygen atom of the ligand and Glu-353 in the ER. This invention reveals a way of increasing the affinity of estradiol position-3 or raloxifene position-6 ether derivatives: replacement of the ether oxygen atom with an amino (NH) group.

In a fourth aspect of this invention, replacement of the 4-hydroxyl group of raloxifene will enhance affinity by picking up a second hydrogen bonding interaction between the amino group and a backbone carbonyl group in Gly-521 of the ER (Fig. 8d).

#### (2) Improved Selectivity

The estrogen receptor has been found to have two discrete forms, known as  $ER\alpha$  and  $ER\beta$ . Furthermore the ratio of the  $\alpha$ - to the  $\beta$ -forms of the ER may vary

considerably in different cell and tissue types. Therefore it may be possible to dissociate desirable therapeutic effects from undesirable side effects of estrogen receptor ligands by designing ligands that selectively bind to one or the other isoforms of the estrogen receptor.

The  $\alpha$ - and  $\beta$ -forms of the estrogen receptor differ significantly in their primary sequence and slightly in their tertiary structure. As a consequence of these receptor differences, ligands may bind with different affinity to the two isoforms.

The present inventors have been able to isolate, differentiate and produce crystals for the ER $\alpha$ . From these crystals, the present inventors have determined the three dimensional structure to high resolution. Further, the inventors have created a partial homology model of ER $\beta$  based on the experimentally derived ER $\alpha$  coordinates. This partial ER $\beta$  homology model captures the essential differences in binding properties between ER $\alpha$  and ER $\beta$ . Based on a comparison of the experimental ER $\alpha$  coordinates and the partial homology model of the ER $\beta$ , the differences between the ER $\alpha$  and ER $\beta$  have been determined and using these differences, the ability of a ligand to bind to either the ER $\alpha$  and ER $\beta$  receptors or to both receptors can be predicted. Hence, if it is known that one tissue possesses solely one form of the estrogen receptor, then it is possible to confer a degree of tissue specificity to a ligand by designing the ligand to bind to that predominant form of the receptor. Advantageously, the ligands may be designed to specifically bind ER $\alpha$  ir ER $\beta$ .

Furthermore, a detailed understanding of the different receptors enables the different behavior of a compound in different tissues to be understood, for example the estrogenic or anti-estrogenic behavior of raloxifen (RAL) dependence on the tissue in which it is active.

Thus, in a further aspect, the invention provides estrogen receptor ligand binding domain crystals for ER $\alpha$  and a partial homology model for ER $\beta$ . Specificity

of ligands for either the ER $\alpha$  and ER $\beta$  or even to a specific ratio of ER $\alpha$  to ER $\beta$  is also provided. The advantage of this is that tissue specificity is conferred to the ligand. Thus, the invention also provides ligands, particularly synthetic ligands of ER $\alpha$  and ER $\beta$  together with methods for their design.

The present invention provides new ligands which exploit these differences by positioning ligand substituents in close proximity to one or more amino acid residue that differ between the  $\alpha$ - and  $\beta$ -isoforms of the ER.

The ligands produced in accordance with the invention bind more effectively to either the  $\alpha$ - or  $\beta$ -isoforms of the ER. The selectivity of the binding between the  $\alpha$ - or  $\beta$ -isoforms may be ten-fold, more preferably one hundred-fold, and most preferably greater than one thousand-fold.

For example, in the  $\beta$ -face cavity of ER- $\alpha$ , the amino acid residue at position-384 is Leu (sidechain volume = 76.6 Å) whereas in the corresponding position of ER- $\beta$ , the amino acid residue is Met (sidechain volume = 79.3 Å<sup>3</sup>). Therefore the  $\beta$ -face cavity of ER- $\beta$  is smaller. Consequently ER- $\alpha$  selectivity may be enhanced by positioning substituents larger than a methyl group in the  $\beta$ -face cavity in close proximity to residue-384. Interaction between the ligand and residue-384 may be enhanced by introducing substituents at the  $\beta$  8-. 15-, or 18-positions on the steroid nucleus.

In the  $\alpha$ -face cavity of ER- $\alpha$ , the amino acid residue at position-421 is Met (sidechain volume = 79.3 Å<sup>3</sup>) whereas in ER- $\beta$ , it is Ile (sidechain volume = 77.3 Å<sup>3</sup>). Therefore the  $\alpha$ -face cavity of ER- $\alpha$  is smaller. This difference may be exploited to produce  $\beta$ -selective compounds through substitutions larger than a methyl group at the  $\alpha$  14-, 16-, or 17-positions of the steroid nucleus.

Similarly, substitutions may be made from either the 2'- or 3'-positions of the 2-arylbenzothiophene nucleus to interact with residue-384 in the  $\beta$ -face cavity or from

the 6'-position to interact with residue-421 in the  $\alpha$ -face cavity (Fig. 9a and 9b). However free rotation about the C2-C1' bond will effectively interchange the substituents at the 2'- and 6'-positions thereby reducing selectivity. Moving the hydroxyl group from position-4' (Fig. 9a) to position-5' (Fig. 9b) will bias the binding orientation such that the  $R_2$  substituent will be positioned in the  $\beta$ -face pocket and the  $R_6$  substituent in the  $\alpha$ -face pocket. This bias results from the fact that only one of the two possible rotamers about the C2'C1' bond will allow hydrogen bond formation between the 5'-hydroxyl group and the receptor residue His-524.

This invention also provides a means of enhancing the selectivity of other classes of non-steroidal ER ligands. In a manner analogous to the benzothiophene series of ER ligands, substituents larger than methyl may be introduced at either the R2' or R3' positions to produced ER- $\alpha$  selective compounds or at R<sub>6</sub>' to produce ER- $\beta$  selective compounds (Fig. 8c).

Substitutions may be made from position-3 of the steroid nucleus or position-6 of the benzothiophene nucleus to exploit the differences between ER- $\alpha$  and ER- $\beta$  at position-326 (Ile in ER- $\alpha$  and Val in ER- $\beta$ ) and at position-445 (Phe in ER- $\alpha$  and Tyr in ER- $\beta$ ).

This invention also provides a means for producing specifically ER- $\alpha$  selective ligands. A six atom linker between the hydroxyl group at position-3 of the A-ring of estradiol or at position-6 raloxifene and an aromatic or heteroaromatic ring on the sidechain will position the sidechain ring in close proximity to residue-445 (Fig. 9c). The edge of ER- $\alpha$  Phe-445 and the face of the sidechain ring can form a favorable " $\pi$ -teeing" interaction. This favorable interaction is not possible with the ER- $\beta$  Tyr-445, therefore analogs of this type with be ER- $\alpha$  selective (Fig. 9d).

Another aspect of this invention provides a means of further enhancing ER- $\alpha$  selectivity. Introduction of a carboxylate or amino group on the meta or para position of the above mentioned aromatic or heteraromatic ring will form a hydrogen bonding

interaction between the conserved Glu-323 or Lys-449 (Fig. 9e). Alternatively, the heteroaromatic ring may be a pyridone ring which will simultaneously form favorable hydrogen bonding interactions with both Glu-323 or Lys-449 (Fig. 9f). Either of the amino, carboxylate, or pyridone ring substitutions will reinforce the favorable " $\pi$ -teeing" interaction between the aromatic or heteroatomic ring of the ligand and Phe-445 in ER- $\alpha$ .

#### (3) Modulation of Efficacy

This invention provides an understanding of the differences between estrogen and antiestrogen binding and therefore a means to design ER ligands with the desired degree of efficacy. An examination of the differences between the ER/estradiol and ER/raloxifene complexes reveals a large movement in Helix-12 (H12, Fig. 6). H12 adopts an "agonistic" conformation defined by the structure of the ER/estradiol complex and an "antagonistic" conformation defined by the structure of the ER/raloxifene complex. These two conformation are in thermodynamic equilibrium. When the ER is complexed with a full agonist, such as estradiol, the equilibrium lies far in the direction of the "agonistic" conformation. In contrast, while when complexed with an antagonist, the equilibrium is pushed in the direction of the "antagonistic" conformation. In the case of raloxifene, the large sidechain at position-3 sterically collides with H12 in it's agonistic conformation, thereby driving the equilibrium strongly in the antagonistic direction. By introduction of progressively shorter sidechains at position-3 of raloxifene, the equilibrium will be gradually shifted back towards the agonist conformation. Thus, this invention provides a means of developing ligands with the desired degree of efficacy (agonist, partial agonist, or antagonist).

In particular, the importance of H12 has been determined as playing a central role in determining the efficacy (agonism vs. antagonism) of a ligand. Thus, ligands which are able to bind to and/or alter the conformation of H12 are of particular importance when designing a ligand or assessing the binding of a ligand, for the

estrogen receptor.

The present inventors have also found the reason why raloxifene has a different binding conformation to that of estradiol, the distinction lying in its active conformation but being unpredictable by virtue of it antagonistic action. The antagonism has been shown, by the present inventors, to be caused by a protruding portion on the raloxifene molecule which causes a large displacement of H12 relative to its conformation in the ER/estradiol complex.

Additionally, it has been found that at least the majority of such receptor proteins are in the form a dimer. Such dimerization leads to a potential route for disruption. Disruptions of this type can be used to predict antagonism or to produce antagonists. Disruptions may take the form of ligand binding which alters the conformation of the helices that comprise the dimerization interface or direct binding to the dimerization interface which then inhibits dimerization.

Further, the orientation of the ligand may be keyed to the receptor, in the dimeric or monomeric form. Furthermore, using the crystals of the present invention, the influence of ligand binding to the LDB on the receptor conformation can now be shown to have influences on the behavior of the receptor since it may disrupt the binding of co-activator, co-repressor, or heat-shock proteins. Previously, such predictions could not me made.

#### Production of estrogen receptor crystals and their application.

Preferably, the crystal is produced from a sequence comprising at least one hundered and fifty amino acids of the selected estrogen receptor. More preferably, the sequence comprises at least two hundred amino acids. Most preferably, the sequence comprises at least two hundred and fifty amino acids. Preferably, the sequence comprises at least a portion of the ligand binding domain of the estrogen receptor.

More preferably, the sequence comprises the whole ligand binding domain of the estrogen receptor.

Typically ER LBDs are purified to homogeneity for crystallization. Purity of ER LBDs is measured with SDS-PAGE, mass spectrometry, and hydrophobic HPLC. The purified ER for crystallization should be at least 97.5% pure, preferably at least 99.0% pure, and most preferably at least 99.5% pure.

Preferably, the crystals used can withstand exposure to X-ray beams used to produce the diffraction pattern data necessary to solve the X-ray crystallographic structure. For example, crystals grown using estrogen receptor sequence bound to a various of ER ligands have been found to decompose during exposure to X-ray beams at room temperature, whereas crystals grown using estrogen receptor sequence bound to various ER ligands are freezable and are able to withstand exposure to X-ray beams.

Advantageously, the crystals have a resolution determined by X-ray crystallography of less than 3.5 Å and most preferably less than 2.8 Å. Preferably crystals grown using naturally occurring estradiol have an effective resolution of lower than 3.1 Å and crystals grown using raloxifene have an effective resolution of lower than 2.6 Å.

The production of such crystals has enabled the three dimensional structure of the ligand binding domain of the estrogen receptor to be mapped. Use of such crystals in conjunction with the map enables a better understanding of how estradiol and other estrogen bind to the estrogen receptor with precision. This technique can also enable the design of estrogen antagonists since the binding site is known.

For example, in the prior art it has been proposed (see Grease et al., J. Med. Chem. (1997), 40:146-147) to prepare raloxifene analogues using a number of substitutions to the 2-aryl group, one of which is 2-napthyl and shows efficacy in

preventing bone loss at the expense of a loss of binding affinity using, for example a 4'-OH substituent (resulting in a slight affinity loss compared to just a napthyl). Having mapped the estrogen receptor, upon reviewing Formula X below, the fit of such a compound into the estrogen binding site comes intuitively apparent, that is, an amalgamation of the D-ring of estradiol and the pendant position-2 aryl substituent, but using the map, the present inventors have found that a 6'-OH, or even a 5'-OH will be more favorable for affinity.

For example, use of such methods has allowed the present inventors to determine the different binding modes of different steroid hormones to the estrogen receptor such as how the binding of testosterone to the estrogen receptor, which is imperfect binding, differs from that of estradiol. In particular, such models show that there is (1) electrostatic repulsion between the C-3 carbonyl oxygen atom of testosterone and the carboxylate of Glu-353 and (2) steric repulsion between the side chain of the C-18 methyl group of testosterone and the side chain of Leu-387 which accounts for the much lower affinity of testosterone compared to estradiol for the estrogen receptor. The steric hindrance and other stereochemical features of molecules has been found to affect the flexibility, that is the ability to alter the tertiary structure, of the ligand binding domain which therefore affects the perturbility of the ligand binding domain. Therefore, using the crystals of the present invention it is now possible for it to be clearly seen how estradiol binds to the estrogen receptor and hence the structural reasons why a compound behaves as an estrogen can not only be understood but also predicted. This enables an understanding of the promiscuity of the estrogen receptor - its ability to bind a variety of structurally diverse ligands. This understanding can be applied to a greater or lesser extent to all steroid hormone receptors, especially the glucocorticoid receptor.

Crystals of the estrogen receptor binding domain can be used as models in methods for the design of synthetic compounds intended to bind to the receptor. Such models show why very slight difference in chemical moieties of a ligand potentially have widely varying binding affinities. Hence, the three dimensional structure of the

ligand binding domain can be used a pharmaceutical model for compounds which bind to estrogen receptors.

Embodiments of the invention will now be described in more detail, by way of example only, with reference to the accompanying drawing Figure 1 to 23 of which:

Figure 1a shows representative portions of a 2.6 Å resolution multicrystal averaged map for a RAL-ER-LBD complex;

Figure 1b is a 3.1 Å resolution six-fold averaged map for a E2-ER-LBD complex. In both Figure 1a and Figure 1b, the map is contoured at 1F and superimposed on the final, refined models;

Figure 2a is a schematic representation of the ER- LBDa indicating the locations of the various secondary structural elements " and 3<sub>10</sub> helices are coloured grey, extended regions are very light grey and coil regions are coloured in dark grey. E2 is coloured very dark grey and is highlighted in space-filling form;

Figure 2b is a topology diagram for ER-LBD. Helices are represented as rectangles and  $\beta$  strands as arrows. The central core layer (H5,H6,H9 and H10 - striped) is sandwiched between the outer flanking layers (H1-4) (H7, H8,H11). The structural elements which flank the layered motif (S1/S2 and H12) are S1, S2, H12 and are cross hatched. The N and C termini are also labelled. All secondary structural elements have been numbered in keeping with the nomenclature that has been established for other known nuclear receptor LBDs;

Figure 3a is a stereoview of the ligand binding cavity. The cavity is viewed in a similar orientation to that given in Fig. 1a. Sidechains for residues that line the cavity are illustrated. Hydrophobic residues are shown in grey, basic residues are shown as spotted and acidic residues are shown in hatched. E2 is coloured black (core) and

dark grey (terminal hydroxyl groups);

Figure 3b is a schematic representation of the ligand binding cavity. Residues that make direct hydrogen bonds to the hydroxyl radius are shown in ball-and-stick representation along with hydrophobic residues that make non-polar interactions with E2 (shown as grey with radial spokes). The atom names and ring nomenclature of E2 are also given;

Figure 3c is a representation of the molecular volume of E2 (dark grey dotted surface) and the accessible binding cavity volume (light grey dotted surface);

Figure 4a is a schematic representations of the ER- $\alpha$  LBD non-crystallographic dimer viewed perpendicular to the dimer axis. The N and C termini are labelled;

Figure 4b is a view of the dimer of Fig. 4a along the dimer axis. E2 is highlighted in mid grey in space-filling form. Helices that are involved in the dimer interface are labelled:

Figure 4c is a view showing the H11 helices that form the backbone of the dimer interface. Interacting residues are show coloured according to polarity (grey -hydrophobic residues; hatched - polar residues; cross-hatched - basic residues);

Figure 5a is a schematic representation of the binding cavity and interactions made by E2. The figure was produced using LIGPLOT software;

Figure 5b is a comparison of the E2 and RAL binding modes (E2 - dark grey; RAL - light grey);

Figure 6 is a schematic representation of the ER-LBD showing the different positioning of helix 12 in the E2 (cross-hatched) and RAL (hatched) complexes. The remainder of the ER-LBD is shown in grey. Dashed lines indicate unmodelled regions

of the structure. The helices which interact with H12 in the two complexes are marked; and

Fig. 7 is a space filling representation of a) an E2 complex and b, an RAL complex. H12 (black) is positioned over the hormone binding cavity in the E2 complex. Raloxifene induces a conformational change so that H12 occupies a hydrophobic groove between H3 and H5. The hydrophobic sidechains of all residues that lie between residues 354 (H3) and 380 (H5) are drawn in dark grey. Other highlighted residues are Lys362 (hatched), Glu380 and Tyr537 (cross-hatched), Asp351 (spots) and the ligand RAL (grey). The remaining atoms of the LBD monomer are white. Note that differences in other parts of the ER-LBD complexes may be due regions missing from the current models;

Fig. 8 shows the structure of several representative estrogen receptor ligands;

Figs. 8a, 8b and 8c show modifications made to the steroid nucleus of ligands which bind to the estrogen receptor;

Figs. 8d and 8e show how affinity of the ligand can be enhanced by adding substituents; and

Figs. 9a-9f show selectivity enhancement by using different substituents on the estrogen receptor ligand; and

Figs. 10 to 19 show by way of structural formulae the chemical reactions involved in the following Examples 1 to 51, which are non-limiting and given by way of illustration only.

Figure 20 shows crystal coordinates for estrogen receptor alpha (ER $\alpha$ ) binding domain in complex with raloxifene.

Figure 21 shows crystal coordinates for estrogen receptor alpha (ERα) binding domain in complex with 17-beta-estradiol.

Figure 22 shows a homology model of estrogen receptor alpha (ER $\alpha$ ) beta complexed with raloxifene.

Figure 23 shows a homology model of estrogen receptor-beta (ER $\beta$ ) complexed with estradiol.

#### **EXAMPLE 1**

#### **Materials**

#### Protein purification and crystallisation of the oestrogen receptor $\alpha$

The human EP-LBD-α was over expressed in Escherichia coli. (Hegy G.B. et al Steroids (1961 61 June 367-373). Fermentation was carried out as batch and fed batch cultivation in a defined glycerol/salt medium at 30°C. Production of recombinant protein was induced by raising the temperature to 39°C. After 2 h, cells were harvested by centrifugation, and frozen, thawed cells were disrupted by a Bead Beater homogenizer (6 x 22 sec., with a 3 min resting time between bursts) (Biospec. Bartlesville, OK, USA), at 0°C, in 100 mM Tris-HC1 (pH 7.8), 100 mM KC1, 10% glycerol, 4mM EDTA, 4 mM DTT, 5µg/ml antipan. For a fermentation volume of 1200 ml, 250 ml buffer was used with 210 ml acid washed glass beads (212-300 microns). After centrifugation, the supernatant was applied to a column of estradiol-Sepharose Fast Flow, 25 ml. (Greene G. et al Proc Natl Acad Sci USA (1980) 77,5115-5119. The column was first washed with 130 ml 10 mM Tris-HCl. (pH 7.8), 700 mM KC1, 1 mM EDTA, followed first by 130 ml 10 mM Tris-HC1 (pH 7.8), 250 mM NaSCN, 10% dimethyl-formamide, 1 mM EDTA and then by 110 ml 10 mM Tris-HC1 pH 8.0. Reactive Cys residues were modified by washing the column with 120 ml 30 mM Tris-base, 15mM iodoacetic acid, pH 8.1. Excess reagent was washed out by 50 ml Tris-base, 15 mM iodoacetic acid, pH 8.1. Excess reagents was washed

out by 50 ml 10 mM Tris-HC1 pH 8.0 followed by 20 ml 10 mM Tris-HC1, ph 7.8, 250 mM NaSCN, 10% dimethylformamide, 1 mM EDTA. The ET-LBD-α was eluted by including 100 μM of the desired ligand to the last buffer. The fractions containing ER-LBD-α was pooled (65 ml) and concentrated (Centriprep 30, Amicon) to 4 ml. Final purification was achieved using a Bio-Rad 491 preparative PAGE instrument according to the user manual. Using one dilution of the Ornstein/Davies buffer system. The stacking (0.7 cm) and resolving (70 cm) gels was 5.6% (acrylamide/bis). The elution buffer was 10mM Tris-HC1 pH 8.0 and the electrophoresis was carried out at 12 W. Fractions containing ER-LBD-α was pooled and concentrated (Centriprep 30) to the desired protein concentration.

#### Data collection, phasing and refinement

#### ER-LBD- $\alpha$ -RAL complex:

A native dataset was collected from a single frozen crystal on beamline X11 at the DESY/Hamburg (1=0.905Å). Diffraction data were recorded at 120K with a 30cm Mar Research image plate located at a crystal-to-detector distance of either 245mm or 390mm. Heavy atom derivatives were collected in-house (York) from flash frozen Data were integrated and reduced using the programs DENZO and SCALPACK. MIR analysis was performed using the CCP4 suite of programs (Table 2). Diffraction data for the alternate C2 (York) and C2221 (DESY, Hamburg) crystal forms were collected to resolutions of 3.0Å and 3.1Å respectively. Initial phases were 3Å using MLPHARE and subsequent two-fold averaging, non-crystallographic matrix refinement and phase extension were carried out using DM. An initial polyalanine trace was used to generate a dimeric search model, using the refined non-crystallographic symmetry and correctly positioned in the alternate C2 and C2221 crystal forms using molecular replacement (AmoRe) Collaborative Computational Project No. 4. (The CCP4 Suite: programs for protein crystallography. Acta Cryst D50, 760-763 (1994)). Twenty cycles of cross crystal averaging between all three crystal forms was carried out with DMMULTI (Supra and Cowtan, K, dm: An automated procedure for phase improvement by density modification. In Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography 31 PP 34-38 (1994)) using only the MIR phase information. The resultant electron density maps showed no bias towards the input model and enabled the unambiguous tracing of the remainder of the molecule and the assignment of most of the amino acid sequence. Refinement was performed with REFMAC using bulk solvent and anisotropic scaling (Murshudou et al Acta Cryst D53, 240-255 (1997)). Tight non-crystallographic restraints were maintained during the initial cycles but were loosened in the final stages of refinement. Individual atomic temperature factors were refined isotropically. Residues Asp332, Phe337, Lys416, Lys467, Ser468, Leu469, Glu470 and Glu471 were poorly resolved in the electron density maps and not modelled beyond their C \$ atoms.

#### ER-LBD- $\alpha$ -E2 complex:

Diffraction data were collected at room temperature from a single ER-LBD-E2 crystal using an 128cm Mar Research image plate located at a crystal-to-detector distance of 280mm on beamline BW7AB at the DESY/Hamburg (l=0.916Å). Initial phase estimates were obtained with AMoRe using the refined ER-LBD RAL dimer (truncated after Met528) as a search model. All data between 15 and 4Å were used for the rotation and translation functions and in the cross-rotation function model Patterson self-vectors were selected within a radius of 30Å. The correct solution, corresponding to three ER-LBD dimers, had a correlation coefficient of 69.8 and an R-factor of 40.6 after AMoRe rigid-body refinement. Six-fold averaging was performed using DM and the structure was refined with REFMAC using tight non-crystallographic restraints, bulk solvent and anisotropic scaling and averaged phases from DM. A single, overall B value was applied in the early stages of refinement until the Rfree converged. Subsequent cycles employed tightly constrained, full isotropic B value refinement. All model building was carried out using the graphics package QUANTA (Molecular Simulations, Inc. San Diego). The sidechains of Leu306, Leu466, Leu 469, Lys492, Lys531 and Leu346 were poorly resolved in the electron density maps and not modelled beyond their C \$ atoms.

TABLE 1

Data collection and refinement statistics

	ER-raloxifene	ER-estradiol
Space group	C2	P21
Unit cell dimensions		
a (Å)	104.53	61.48
B (Å)	53.68	115.16
C (Å)	102.71	137.38
β (ο)	116.79	103.01
No. of molecules / AU	2	6
Resolution (Å)	25 - 2.6	20 - 3.1
No. unique reflections	15,497	34,025
Completeness (%)	94.6	99.1
Multiplicity	4.5	2
Rsym (I)	8	10
Reflections used in	13,868	30,583
refinement		
Rcryst	23.98	22
Rfree	30.4	25.3
Non H atoms	3,741	11,508

Water	66	126
% A.B,L (a,b,l,p)	92.4 (7.6)	93.0 (7.0)
Rmsd bond length (Å)	0.01	0.01
Rmsd bond angle (Å)	0.04	0.03
Average B protein (Å2)	48.3	37.8
Rmsd NCS protein (Å)	0.57	0.08
Rmsd NCS B (Å2)	8.2	1.1

Rsym (I) =  $100x G_hG_i1G_{hi}$ -<I> $>1/G_hG_iI_{h..i}$  where I is the observed intensity. <I> is the average intensity of multiple observations of symmetry related reflections.

Reryst =  $100 \times E11F_01-1F_c11/E1f_01...$ 

Rfree is the same as Rcryst but was calculated using a test set of reflections (10% of the whole dataset) that was excluded from the refinement process.

R.m.s. deviation in bond length and the angle distances from Engh and Huber ideal values

R.m.s. distance between all non-crystallographic symmetry (NCS) related atom positions

R.m.s. difference between all non-crystallographic symmetry (NCS) related atomic temperature factors.

TABLE 2

Heavy atom data collection and MIR statistics

Dataset	PCMBS-1	PCMBS-2	KAuCN
Resolution (Å)	20 -3	20 -3	20 -3.6

PCT/GB98/01708

No. unique reflections	10,335	9,316	5,835
Completeness (%)	97.6	89	94.2
Multiplicity	4	3.1	2.5
Rsym (I)	8.1	9.2	7
Conc. reagent (mM)	4	4	4
Soak time (days)	5	14	2
Resolution (Å)	20 -3	20 -3	20 -3.6
Riso	16.9	20.7	13.7
No. of sites	2	2	1
Cullis R (centric / acentric)	0.75/0.68	0.76 / 0.66	0.90 / 0.85
Phasing power (centric / acentric)	1.22 / 1.88	1.23 / 2.02	0.71 / 0.94
F.O.M (20 - 3Å) (centric / acentric / overall)		0.67 / 0.48 / 0.49	·

Cullis R =E1E1/G11F<sub>PH</sub> 1-1FP<sub>P</sub>11 for centric (c) and acentric (a) reflections. F.O.M =  $\langle EP(\alpha)e^{i\alpha}/EP(\alpha)\rangle$  where  $\alpha$  is the phase and  $P(\alpha)$  is the phase probability distribution. Phasing power.

#### **EXAMPLE 2**

#### ER -E2 crystallisation

Prior to crystallisation protein was buffer exchanged to 20 mM using Tris/HC1 buffer at pH 7.8 and concentrated to 12-13 mg/ml. Crystals were grown by vapour diffusion using hanging and sitting drop techniques. The best crystals were obtained using 2.4 M Ammonium formate or 80-90 mM Magnesium formate as precipitants buffered with 0.1 M Tris/HC1 buffer. 4 M Ammonium formate or 200 mM Magnesium formate unbuffered stock solutions were used. Magnesium formate stock solution was kept at 4°C and filtered before use. The optimum pH ranged from 7.9 to 8.3 with the best crystals growing at pH 8.1. Protein concentration in the drop was 8 mg/ml although X-ray suitable crystals were also obtained at 13 mg/ml. However, crystals obtained from such conditions were very often twinned and the addition of DMSO at up to 8% significantly improved their quality. The size of the crystals was correlated with the size of the sitting/hanging drop. The optimum size of the drop was achieved by mixing 2.5 ml of protein with 2.5ml of the reserved solution. All crystallisations were performed at 18°C. The best crystals, with a size of 0.5x0.05x0.05 mm<sup>3</sup>, were mounted in the X-ray quartz capillaries.

#### ER-α-Raloxifen (ER-R) crystallisation

After purification as before, the protein buffer was replaced with 20 mMTris/HCl pH 7.8-7.9 and the protein was concentrated usually to 10-12 mg/ml. The vapour diffusion method with the hanging drop technique was used for crystallations. The best conditions for crystallisation used the following medium: 0.1 M Tris/HCl buffer pH 8.3, 12% (w/v) of PEG 4000, 0.1 M Maltose, 50 mM Lysine, 0.2 M MgCl2, 5% dioxane. The concentration of the protein solution used for crystallisation was brought up to 7.3-7.5 mg/ml by dilution with 20 mM Tris/HCl buffer pH 8.3. Cyrstallisations were performed with different drop sizes and protein-to-reservoir buffer ratios. The

best crystals were grown from drops obtained by mixing 2 ml of protein with 2 ml or 3 ml of well buffer. The best temperature for crystal growth is 18°C. These conditions yielded the main C2 crystal form (a=104.53Å b=53.68Å c=102.71Å b=116.79Å, in the shape of monoclinic plates (0.1x0.1x0.02 mm<sup>3</sup>)), which was subsequently used for heavy atoms derivatives searches and structure refinement.

By subtle manipulation of the above conditions other crystal forms were also produced. The lowering of the PEG 4000 concentration to 10-11 % w/v resulted in other C2 crystal form: a=89.9Å b=75.09Å c=87.50Å b=103.01o. These crystals grow at 18°C as single pyramids and despite their severe twinning it was possible to separate mechanically small untwinned fragments of the crystals suitable for X-ray data collection.

The alteration of other conditions, for example increase of dioxan concentration from 5 to 7.5 and 10% and replacement of 50 mM Lys by 50 mM Arg, 0.1 M Maltose by 0.1 M Sucrose or Glucose, produced C2221 orthorhombic crystal form: a=65.47Å b=95.99Å c=164.14Å Crystals reached the size of 0.2x0.03x0.03 mm3 and they were growing preferably at 18°C.

It is also possible to obtain crystals of SeMet derivative or ER-R complex. They can be grown from conditions typical for the main C2 crystal form, but the concentration of dioxan is raised usually up to 7.5%. These crystals were very fragile and give poor quality X-ray data: which was used as additional information for positioning Met residues only.

All ER-RAL complex crystal forms were suitable for flash-cooling by using a stream of  $N_2$  at 100 K and 120 K. In all cases, the cryoprotectant consisted of mother liquor (well buffer composition) and 25% v/v MPD.

Owing to the sensitivity of the ER-R crystals all heavy atoms soaks were done in the exact mother liquor (taken from the well buffer) and the heavy atoms compounds were

always dissolved as a solid substance in these solutions. PCMBS-1 and KAuCN soaks were done for three days, PCMBS-2 for three weeks. All soaks done at 18°C. The cryo-solutions contained the heavy atom compounds at soaking concentration as well.

Pure ER-LBD is particularly refractive to crystallisation and suitable crystals were obtained after carboxymethylation of the three thiol groups.

#### **EXAMPLE 3**

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#### Structure Determination of the Estrogen Receptor α-Ligand Binding Domain

Crystals of the ER "-LBD complexed with either estradiol or raloxifen will diffract to medium resolution, are monoclinic and contain either a single dimer in the case of raloxifen or three dimers in the case of estrogen in the asymmetric unit (see Table 1), Multiple isomorphous replacement was used to determine the crystal structure of the ER-LBD-RAL complex. An initial multiple isomorphous replacement/density modified electron density map showed the position of the non-crystallographic two-fold rotation axis and allowed an initial polyalanine trace to be built on the resultant two-fold averaged map. Subsequent averaging between three different crystal forms of the RAL complex enabled corrections to be made to the initial trace. The remainder of the protein as yet not being unambiguously traced and most of the amino acid sequence to be assigned. The resultant model had an R value of 43%. Cycles of maximum likelihood refinement and manual rebuilding yielded a final model with acceptable R values and geometric parameters. The initial phase estimates were obtained for the estradiol (E2) complex by molecular replacement using the ER-LBD RAL dimer as a search model. Rotation in translation functions yielded the correct solution. Six-fold averaging between the three dimers in the crystal line asymmetric unit allowed both the missing parts of the structure to be traced and the positioning of E2 in the binding cavity to be determined. The structure was refined using both tight non-crystallographic restraints as well as average phase information to yield a final model with an Rcryst of 22.0 and R3 of 25.3 for all data between 20 and 3.1 ® (Table 1).

#### Results

The crystals produced in Example I and II were subjected to X-ray crystallographic studies which revealed that the LBD is folded into a characteristic "wedge-shaped" globular unit. It has a three-layered, anti-parallel \alpha-helical sandwich motif and is constructed from 8 major helices The motif comprises a central core layer of 3 helices (H5/6, H9 and H10) sandwiched between two additional layers of helices (H2-3 and H7, H8, H11). The arrangement of structural elements in this fashion creates a "molecular scaffold" maintaining a sizable ligand binding cavity at the "toe end" of the wedge-shaped domain. The remaining secondary structural elements, a small two stranded anti-parallel β-sheet (S1 and S2) and helix H12, are located at the "ligand binding end" of the molecule and flank the main three-layered motif (see Figure 2). From the N-terminus, the chain follows one turn of the distorted "-helix (H1), turns 90° and enters a short helix (H2) that lies parallel to the longest axis of the LBD. After helix H2, the chain continues in the same direction in an irregular extended conformation before tucking under the bottom of the molecule. At this stage, the chain turns back on itself through the long, bent, helix (H3). N-terminal portion of this helix forms part of the ligand binding cavity. The sequence has a proline at position 365 which is invariable and it is at this residue that the main chain takes a sharp (90°) change in direction, passes through a 310 helix (H4) before forming the first of three central helices (H5/6). Helix H5/6 can be geometrically described as a single unit, although it is kinked by 40° at the alanine residue at position 382 in a manner such that its C-terminal end is correctly positioned to form part of the E2 binding cavity. This helix is kinked and is distinguishing and is maintained by a series of hydrophobic interactions between leucines at 378 and 379 (H5) with a phenol at 367 and leucine at 453 all of which are highly conserved and are part of the nuclear receptor LBD signature motif (Wurst). From this position the sequence passes through a small \$\hairpin (S1/S2) covering one side of the binding cavity, and emerges on the other side of the molecule via the 3<sub>10</sub> helix H7. Helix H8 runs three quarters of the way up the long axis of the LBD, passes through a second central helix (H9) before turning back via a disordered loop to form a final helix H10.

At the end of H10, the polypeptide backbone changes direction and runs the full length of the ligand binding domain, in an anti-parallel direction to H8 in the form of helix 11. After a short turn the chain emerges on the opposite side to the S1/S2  $\beta$  hairpin at helix H12, the core amphipathic helix of the AF-2 region.

#### **DIMERISATION**

Crystallographic studies also reveal that the receptor is dimerised. ER is sequestered in an inactive complex with heat shock protein 90 (hsp90) and other accessory factors in the absence of E2. Ligand binding initiates the disassembly of this complex and results in receptor dimerisation via domain E. The ligand-bound form of ER exists as a tight homodimer in solution and ER-LBDs are arranged as non-crystallographic dimers within both the E2 and RAL complex crystals. This quaternary arrangement almost certainly reflects the physiological state of ER-LBD in vivo as all crystal forms of the liganded ER-LBD obtained to date contained non-crystallographic dimers. The dimer axis coincides with the longest axis of the LBD with each molecule tilted approximately 15° away from the two position fold. This symmetric arrangement generates a molecule with dimensions of approximately 55Å high by 50Å wide by 35-60Å breadth. The observed quaternary arrangement locates the N and C termini of each monomer on the opposite "faces" of the dimer. The C terminus of each monomer projects towards the dimer axis while the N termini are far removed from the interface. The dimerisation surface is fairly extensive and encompasses about 15% (1,703 Å<sup>2</sup>) of each monomer's accessible surface area. The LBD's are positioned so that the H8/H11 face of each monomer lines up to form an additional, intermolecular helical layer. Contacts between the two molecules are made primarily through the H11 helices, which intertwine to form a rigid backbone, but also involve H8 from one monomer and H9 and H10 from the neighbouring monomer. The H11 helices are arranged as a bifurcated coiled coil with the side chains of the residues Leu 504, Ala 505. Leu 508, Leu 509 and Leu 511 which are interdigitated to form a partial "leucine zipper" motif at the coils end terminal N. This hydrophobic patch is flanked on either side by a network of hydrogen bonding residues. Arg 545 and Asn 519 make direct hydrogen bonds with Ser 512 and His 516 respectively. This overall monomer-monomer arrangement is unaffected by the nature of the ligand and seems to be maintained within the receptor super family. The observed ER-LBD dimer is identical in terms of gross monomer orientation and make up of the dimer interface to that of the crystallographic unliganded RXR- $\alpha$  homodimer (58% hydrophobic/42% hydrophillic).

The invariable nature of the LBD's quaternary structure therefore suggests that it provides a stable entity that facilitates separation of the two DNA binding domains in such a way as to allow optimal binding to EREs.

Such an elucidation of the 3-dimensional structure of the estrogen receptor ligand binding domain provides a useful tool for designing ligands for binding to the estrogen receptor. Such a detailed knowledge of the structure of the receptor enables prediction with accuracy whether a ligand binding to the receptor will act as an antagonist, a partial antagonist, an agonist or a partial agonist since the ligand-induced conformational changes can be anticipated.

#### **EXAMPLE 4**

#### Partial Homology Model of ERB

The coordinates obtained in Example I (ERα complexed with either estadiol or with raloxifine) were used to create two partial homology models of ERβ (complexed with estradiol and raloxifene respectively). This was accomplished by importing the ERα coordinates into version 6.4 of Sybyl (available from Tripos Associates, St. Louis, MO, U.S.A.). The "change" command in the Sybyl biopolymer module was used to mutate amino acids which differ between ERα and ERβ and which are in the vicinity of the ligand binding pocket. Four such residues were mutated: 1326V (Ile-326 to Val), L384M (Leu-384 to Met), M421I (Met-421 to Ile), F445Y (Phe-445 to Tyr). These partial ERβ homology models in conjunction with the experimental ERα coordinates were used to design isoform selective ligands as described in Example 5-51.

#### **Design of Ligands**

Examples of ligands designed to fit the receptor have been produced as follows:

#### Example 5

#### 2-(2,6-dimethylphenyl)-6-hydroxybenzo[β]thiophene (1).

- (a) To a solution of 6-methoxybenzo[β]thiophene (Graham et al, J. Med. Chem., 1989, 32, 2548.) (6 g, 36.5 mmol) in 50 ml of anhydrous tetrahydrofuran at -60°C was added n-butyllithium (20.5 ml, 41 mmol, 2.0 M solution in cyclohexane), dropwise via a dropping funnel. After stirring for 30 minutes, trimethyltin chloride (41 ml, 41 mmol, 1.0 M solution in hexanes) was introduced dropwise through a dropping funnel. The resulting mixture was allowed to warm to 0°C, stirred for 1 hour and then quenched with 100 ml of 1 M hydrochloric acid. The aqueous phase was extracted with ethyl acetate. The combined organic phases were dried over sodium sulphate and then concentrated in vacuo. This produced 9.24 g (28 mmol, 77%) of 2-trimethylstannyl-6-methoxybenzo[β]thiophene as white semicrystals. <sup>1</sup>H NMR (CDCl<sub>3</sub>) 7.66 (d, J = 8.6 Hz, 1H), 7.34 (d, J = 2.2 Hz, 1H), 7.29 (s, 1H), 6.95 (dd, J = 8.6 Hz, 2.2 Hz, 1H), 3.86 (s, 3H), 0.39 (s, 9H).
- (b) A mixture of 370 mg (2 mmol) 2-bromo-m-xylene, 115 mg (0.1 mmol) tetrakis triphenylphosphinepalladium (0) and 160 mg (2 mmol) of cupric oxide in 8 ml of N,N-dimethylformamide was stirred at 100°C under nitrogen. After 5 minutes, 981 mg (3 mmol) of 2-trimethylstannyl-6-methoxybenzo[β]thiophene (example 1a) in 2 ml of N,N-dimethylformamide was added all at once to the reaction mixture. The reaction was heated for 2 hours and then allowed to reach room temperature. The resulting mixture was concentrated, dissolved in ethylacetate, filtered through a pad of silica and concentrated. The crude product was purified on a chromatotron (silica, 99:1, petroleum ether/ethyl acetate) producing 328 mg (1.22 mmol, 61%) of 2-(2,6-dimethylphenyl)-6-methoxybenzo[β]thiophene a yellowish crystals. H NMR (CDCl<sub>3</sub>) 7.89 (d, J = 8.7 Hz, 1H), 7.32-7.59 (m, 4H), 7.23 (dd, J = 8.7 Hz, 2.2 Hz, 1H), 7.18 (s, 1H), 4.12 (s, 3H), 2.46 (s, 6H).

(c) 145 mg (0.54 mmol) of 2-(2,6-dimethylphenyl)-6-methoxybenzo[β]thiophene (example 1b) was dissolved in 15 ml of dichloromethane, to the stirred solution was added boron trifluoride dimethylsulfide complex (1.5 ml). The solution was stirred at room temperature under nitrogen in the dark for 15 hours. The reaction mixture was quenched with 10 ml of water, extracted with dichloromethane, dried over magnesium sulphate and concentrated. The crude product was purified on a chromatotron (silica, 80:20, petroleum ether/ ethyl acetate) producing 94.1 mg (0.37 mmol, 69%) of 2-(2,6-dimethylphenyl)-6-hydroxybenzo[β]thiophene as white crystals. MP 95-96°C. <sup>1</sup>H NMR (CDCl<sub>3</sub>) 7.63 (d, J = 8.6, 1H), 7.08-7.31 (m, 4H), 6.92 (s, 1H), 6.91 (dd, J = 8.6, 2.2 Hz, 1H), 4.91 (s, 1H), 2.20 (s, 6H).

#### Example 6

#### 2-(2-ethyl-6-methylphenyl)-6-hydroxybenzo[β]thiophene (2).

- (a) The cross-coupling of 492 mg (2 mmol) 2-ethyl-6-methyliodobenzene, with 981 mg (3 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 99:1, petroleum ether/ ethyl acetate) producing 438 mg (1.55 mmol, 78%) of 2-(2-ethyl-6-methylphenyl)-6-methoxybenzo[ $\beta$ ]thiophene as a colourless oil. <sup>1</sup>H NMR (CDCl<sub>3</sub>) 7.67 (d, J = 8.9 Hz, 1H), 7.08-7.36 (m, 4H), 7.01 (dd, J = 8.9 Hz, 2.2 Hz 1H), 6.96 (s, 1H), 3.89 (s, 3H), 2.54 (q, J = 7.6 Hz, 2H), 2.19 (s, 3H), 1.12 (t, J = 7.6 Hz, 3H).
- deprotection 100 (b) o f m g (0.35)mmol) o f 2-(2-ethyl-6-methylphenyl)-6-methoxybenzo[β]thiophene (example 2(a)was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 90:10, petroleum ether/ ethyl acetate) producing 69 mg (0.26 mmol, 73%) of 2-(2-ethyl-6-methylphenyl)-6-hydroxybenzo[β]thiophene as white semicrystals. <sup>1</sup>H NMR (CD<sub>3</sub>OD) 7.59 (d, J = 8.7, 1H), 7.06-7.25 (m, 4H), 6.90 (s, 1H), 6.88 (dd, J = 8.7, 2.2 Hz, 1H), 2.51 (q, J = 7.6 Hz, 2H), 2.15 (s, 3H), 1.09

(t, J = 7.6 Hz, 3H).

#### Example 7

2-(2.6-dimethyl-4-hydroxyphenyl)-6-hydroxybenzo[β]thiophene (3).

- (a) The cross-coupling of 402 mg (2 mmol) 4-bromo-3,5-dimethylphenol, with 981 mg (3 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 90:10, petroleum ether/ ethyl acetate) producing 210 mg (0.74 mmol, 37%) of 2-(2,6-dimethyl-4-hydroxyphenyl)-6-methoxybenzo[ $\beta$ ]thiophene as yellow crystals. HNMR (CDCl<sub>3</sub>) 7.88 (d, J = 8.7 Hz, 1H), 7.55 (d, J = 2.5 Hz, 1H), 7.22 (dd, J = 8.7 Hz, 2.5 Hz 1H), 7.14 (s. 1H), 6.83 (s, 2H), 4.94 (s, 1H), 4.11 (s, 3H), 2.38 (s. 6H).
- (b) The deprotection of 100 mg (0.35 mmol) of 2-(2.6-dimethyl-4-hydroxyphenyl)-6-methoxybenzo[ $\beta$ ]thiophene (example 3(a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 80:20, petroleum ether/ethyl acetate) producing 52 mg (0.19 mmol, 54%) of 2-(2,6-dimethyl-4-hydroxyphenyl) -6-hydroxybenzo[ $\beta$ ]thiophene as white crystals. MP 202-204°C, <sup>1</sup>H NMR (CD<sub>3</sub>OD) 7.56 (d, J = 8.7, 1H), 7.19 (d, J = 2.2 Hz, 1H), 6.86 (dd, J = 8.7, 2.2 Hz, 1H), 6.84 (s, 1H), 6.54 (s, 2H), 2.10 (s, 6H).

#### Example 8

- 2-(2-methylphenyl)-6-hydroxybenzo[ $\beta$ ]thiophene (4).
- (a) The cross-coupling of 340 mg (2 mmol) 2-bromotoluene, with 981 mg (3 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b) The crude product was purified on a chromatotron (silica, 99:1, petroleum ether/ethyl acetate) producing 500 mg (1.97 mmol, 98%) of

2-(2-methylphenyl)-6-methoxybenzo[ $\beta$ ]thiophene as white crystals. <sup>1</sup>H NMR (CDCl<sub>3</sub>) 7.66 (d, J = 8.7 Hz, 1H), 7.19-7.49 (m, 5H), 7.15 (s, 1H), 6.99 (dd, J = 8.7, 2.3 Hz, 1H), 3.88 (s, 3H), 2.48 (s, 3H).

(b) The deprotection of 125 mg (0.49 mmol) of 2-(2-methylphenyl) -6-methoxybenzo[ $\beta$ ]thiophene (example 4(a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 90:10, petroleum ether/ ethyl acetate) producing 60 mg (0.23 mmol, 47%) of 2-(2-methylphenyl)-6-hydroxybenzo[ $\beta$ ]thiophene as white crystals. MP 97-98°C, <sup>1</sup>H NMR (CDCl<sub>3</sub>) 7.63 (d, J = 8.4 Hz, 1H), 7.18-7.48 (m, 5H), 7.14 (s, 1H), 6.91 (dd, J = 8.4, 2.3 Hz, 1H), 4.86 (s, 1H), 1.56 (s, 3H).

#### Example 9

 $2-(2-chloro-6-methylphenyl)-6-hydroxybenzo[\beta]thiophene (5).$ 

- (a) The cross-coupling of 505 mg (2 mmol) 3-chloro-2-iodotoluene, with 981 mg (3 mmol) of product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 99:1, petroleum ether/ethyl acetate) producing 439 mg (1.52 mmol, 76%) of 2-(2-chloro-6-methylphenyl) -6-methoxybenzo[β]thiophene as a yellow oil. <sup>1</sup>H NMR (CDCl<sub>3</sub>) 7.68 (d, J = 8.7 Hz, 1H), 7.15-7.36 (m, 4H), 7.03 (s, 1H), 7.01 (dd, J = 8.7, 2.2 Hz, 1H), 3.88 (s, 3H), 2.25 (s, 3H).
- (b) The deprotection of 100 mg (0.35 mmol of 2-(2-chloro-6-methylphenyl) -6-methoxybenzo[ $\beta$ ]thiophene (example 5(a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 90:10, petroleum ether/ ethyl acetate) producing 44 mg (0.16 mmol, 46%) of -2-(2-chloro-6-methylphenyl)-6-hydroxybenzo[ $\beta$ ]thiophene as a yellowish oil. <sup>1</sup>H NMR (CD<sub>3</sub>OD) 7.62 (d, J = 8.7 Hz, 1H), 7.18-7.35 (m, 4H), 6.99 (s, 1H), 6.89 (dd, J = 8.7, 2.2 Hz, 1H), 2.23 (s, 3H).

## Example 10

## 2-(2-methylnaphth-1-yl)-6-hydroxybenzo[ $\beta$ ]thiophene (6).

- (a) The cross-coupling of 221 mg (1 mmol) 1-bromo-2-methylnaphthalene, with 491 mg (1.5 mmol) of product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 99:1, petroleum ether/ ethyl acetate) producing 159 mg (0.52 mmol, 52%) of 2-(2-methylnaphth-1-yl)-6-methoxybenzo[ $\beta$ ]thiophene as white crystals. <sup>1</sup>H NMR (CDCl<sub>3</sub>) 7.66-7.88 (m, 4H), 7.30-7.48 (m, 4H), 7.11 (s, 1H), 7.04 (dd, J = 8.7, 2.2 Hz, 1H), 3.91 (s, 3H), 2.40 (s, 3H).
- (b) The deprotection of 110 mg (0.36 mmol) of 2-(2-methylnaphth-1-yl) -6-methoxybenzo[β]thiophene (example (6a)) was accomplished b the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 90:10, petroleum ether/ethyl acetate) producing 52 mg (0.18 mmol, 50%) of -2-(2-methylnaphth-1-yl)-6-hydroxybenzo[β]thiophene as white semi crystals. HNMR (CD<sub>3</sub>COCD<sub>3</sub>) 8.60 (s, 1H) 7.87-8.05 (m, 2H), 7.74 (d, J = 8.7 Hz, 1H), 7.65-7.71 (m, 1H), 7.38-7.54 (m, 4H) 7.18 (s, 1H), 7.02 (dd, J = 8.7, 2.2 Hz, 1H), 2.39 (s, 3H).

#### Example 11

## 2-(2,5-dimethyl-4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ]thiophene (7).

(a) The cross-coupling of 248 mg (1 mmol) 2,5-dimethyl-4-iodophenol, with 491 mg (1.5 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 9:1, petroleum ether/ ethyl acetate) producing 130 mg (0.46 mmol, 46%) of 2-(2,5-dimethyl-4-hydroxyphenyl)-6-methoxybenzo[β]thiophene as white crystals. <sup>1</sup>H NMR (CDCl<sub>3</sub>) 8.34 (s, 1H), 7.69 (d, J = 8.8 Hz, 1H), 7.45 (d, J = 2.3 Hz, 1H), 7.19 (s, 1H), 7.17 (s, 1H), 6.98 (dd, J = 8.8, 2.3 Hz, 1H), 6.78 (s, 1H), 3.87 (s, 3H), 2.34

(s, 3H), 2.20 (s, 3H).

(b) The deprotection of 35 mg (0.12 mmol) of 2-(2,5-dimethyl -4-hydroxyphenyl)-6-methoxybenzo[β]thiophene (example (6a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 70:30, petroleum ether/ ethyl acetate) producing 26 mg (0.096 mmol, 80%) of 2-(2,5-dimethyl-4-hydroxyphenyl)-6-hydroxybenzo[β]thiophene as white crystals. MP 134-136°C, <sup>1</sup>H NMR (CD<sub>3</sub>COCD<sub>3</sub>) 8.41 (s broad, 2H) 7.63 (d, J = 8.7 Hz, 1H), 7.30 (d, J = 2.2 Hz, 1H), 7.18 (s, 1H), 7.13 (s, 1H) 6.93 (dd, J = 8.7, 2.2 Hz, 1H), 6.77 (s,1H), 2.34 (s, 3H), 2.19 (s, 3H).

Example 12

2-(4-hvdroxyphenyl)-6-hydroxybenzo[β]thiophene (8).

Prepared according to (Hauser et al, WO 96/30361).

Example 13

2-(2-benzylphenyl)-6-hydroxybenzo[ $\beta$ ]thiophene (9).

The cross-coupling of 124 mg (0.5 mmol) 2-bromodiphenylmethane, with 246 mg (0.75 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was deprotected by the procedure set forth in example 1 (c). It was purified on a chromatotron (silica, 92:8, petroleum ether/ ethyl acetate) producing 108 mg (0.34 mmol, 68%) 2-(2-benzylphenyl) -6-hydroxybenzo[β]thiophene as slightly pink crystals. H NMR (CD<sub>3</sub>COCD<sub>3</sub>) 8.55 (s 1H) 7.62 (d, J = 8.4 Hz, 1H), 7.04-7.51 (m, 11H), 6.93 (dd, J = 8.5, 2.5 Hz, 1H), 4.19 (s, 2H).

Example 14

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Example 14

2- $(4-hydroxynapht-1-yl)-6-hydroxy[\beta]thiophene (10)$ 

The cross-coupling of 119 mg (0.5 mmol) 1-bromo-4-methoxynaphthalene, with 246 mg (0.75 mmol) of the product from  $\mathbf{1}(a)$  was accomplished by the procedure set forth in example  $\mathbf{1}(b)$ . The crude product was deprotected by the procedure set forth in example 1 (c). It was purified on a chromatotron (silica, 8:2, petroleum ether/ ethyl acetate) producing 9 mg (0.03 mmol, 6.2%) 2-(4-hydroxynapht-1-yl)-6-hydroxy[ $\beta$ ]thiophene(10) as dark brown crystals. HNMR (CD<sub>3</sub>COCD<sub>3</sub>) 9.34 (s, 1H), 8.55 (s 1H), 8.31-8.38 (m, 1H), 8.20-8.27 (m, 1H), 7.72 (d. J = 8.4 Hz, 1H), 7.48-7.58 (m, 2H), 7.48 (d, J = 7.7, 1H), 7.37 (d, J = 2.2, 1H), 7.34 (s, 1H), 7.00 (d, J = 7.7, 1H), 6.98 (dd, J = 8.4, 2.2 Hz, 1H).

Example 15

## 2-(2-methyl-3-chlorophenyl)-6-hydroxybenzo[ $\beta$ ]thiophene (11).

The cross-coupling of 126 mg (0.5 mmol) 2-chloro-6-iodotoluene, with 246 mg (0.75 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was deprotected by the procedure set forth in example 1 (c). It was then purified on a chromatotron (silica, 92:8, petroleum ether/ethyl acetate) producing 88 mg (0.32 mmol, 64.1%) of 2-(2-methyl-3-chlorophenyl)-6-hydroxybenzo[β]thiophene (11). HNMR (CDCl<sub>3</sub>) 7.72 (d, J = 8.7 Hz, 1H), 7.29-7.41 (m, 2H), 7.27 (d, J = 2.5, 1H), 7.17 (d, J = 7.91, 1H), 7.10 (s, 1H), 6.92 (dd, J = 8.7, 2.5 Hz, 1H), 2.46 (s, 3H).

Example 16

## 2-(2-methyl-5-chlorophenyl)-6-hydroxybenzo[β]thiophene (12).

The cross-coupling of 126 mg (0.5 mmol) 4-chloro-2-iodotoluene, with 246 mg (0.75 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was deprotected by the procedure set forth in example 1 (c). It was then purified on a chromatotron (silica, 92:8, petroleum ether/ethyl acetate) producing 88 mg (0.32 mmol, 64.1%) of 2-(2-methyl-5-chlorophenyl) -6-hydroxybenzo[β]thiophene (12). <sup>1</sup>H NMR (CDCl<sub>3</sub>) 7.63 (d, J = 8.7 Hz, 1H), 7.43 (d, J = 2.0 Hz, 1H), 7.27 (d, J = 2.2, 1H), 7.19-7.23 (m, 2H), 7.14 (s, 1H), 6.92 (dd, J = 8.5, 2.2 Hz, 1H), 2.41 (s, 3H).

#### Example 17

# 2-(2-methyl-4-chlorophenyl)-6-hydroxybenzo[ $\beta$ ]thiophene (13).

The cross-coupling of 103 mg (0.5 mmol) 2-bromo-5-chlorotoluene, with 246 mg (0.75 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was deprotected by the procedure set forth in example 1 (c). It was then purified on a chromatotron (silica, 92:8, petroleum ether/ethyl acetate) producing 118 mg (0.43 mmol, 85.9%) 2-(2-methyl-4-chlorophenyl) -6-hydroxybenzo[β]thiophene (13) as slightly pink crystals. <sup>1</sup>H NMR (CD<sub>3</sub>COCD<sub>3</sub>) 8.63 (s. 1H), 7.69 (d, J = 8.7 Hz, 1H), 7.45 (d, J = 8.4 Hz, 1H), 7.26-7.41(m, 4H), 6.92 (dd, J = 8.4, 2.2 Hz, 1H), 2.47 (s, 3H).

## Example 18

## 2-(2.5-hydroxy-4-bromophenyl)-6-hydroxybenzo[β]thiophene (14).

The cross-coupling of 222 mg (0.75 mmol) 1,4-dibromo-2,5-dimethoxybenzene with 367 mg (1.125 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). It was then purified on a chromatotron (silica, 95:5, petroleum ether/ acetone) producing 65.5 mg (0.17 mmol, 23%) of 2-(2.5-methoxy-4-bromophenyl)-6-methoxybenzo[\beta]thiophene. 25 mg (0.066 mmol)

14.1 mg (0.042 mmol, 63.4%) of 2-(2,5-hydroxy-4-bromophenyl) -6-hydroxybenzo[ $\beta$ ]thiophene. <sup>1</sup>H NMR (CD<sub>3</sub>COCD<sub>3</sub>) 8.84 (s, 1H), 8.54 (s, 1H), 8.33 (d, J = 8.74 Hz, 1H), 7.81 (s, 1H), 7.69 (d, J= 8.4 Hz, 1H), 7.34 (d, J = 2.2 Hz, 1H), 7.28 (s, 1H), 7.14 (s, 1H), 6.92 (dd, J = 8.4, 2.2 Hz, 1H).

## Example 19

## 2-(2-methyl-4-nitrophenyl)-6-hydroxybenzo[ $\beta$ ]thiophene (15).

- (a) The cross-coupling of 432 mg (2.0 mmol) 2-bromo-5- nitrotoluene with 982 mg (3.0 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 8:2, petroleum ether/ ethyl acetate) producing 681 mg (about 75% pure) of 2-(2-methyl-4-nitrophenyl)-6-methoxybenzo[β]thiophene.
- (0.33)mmol) 2-(2-methyl-4deprotection of 100 mg (b) The nitrophenyl)-6-methoxybenzo[β]thiophene (example (15a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 70:30, petroleum ether/ ethyl acetate) producing 73 mg (0.26 mmol, 78%) of 2-(2-methyl-4-nitrophenyl)-6-hydroxybenzo[β]thiophene. H NMR (CDCl<sub>3</sub>) 8.16 (d broad, J = 2.1 Hz, 1H) 8.08 (dd, J = 8.5, 2.1 Hz, 1H), 7.68 (d, J = 8.5 Hz, 1H), 7.60 (d, J = 8.5, 1H), 7.29 (d, J = 2.4 Hz, 1H) 7.27 (s, 1H), 6.94 (dd, J = 8.5, 2.4 Hz, 1H),5.15 (s, 1H), 2.59 (s, 3H).

## Example 20

# 2-(2-methyl-4-aminophenyl)-6-hydroxybenzo[ $\beta$ ]thiophene (16).

50 mg (0.18 mmol) of 2-(2-methyl-4-nitrophenyl) -6-hydroxybenzo[β]thiophene (example (15(b)) was dissolved in 5 ml of ethanol and 198 mg (0.88 mmol) of tin dichloride dihydrate was added. The mixture was heated to 70°C under a nitrogen

atmosphere for 3 hours. Hydrochloric acid (1 M) was added and then the aqueous phase was extracted with ethyl acetate. The combined organic phases were washed with brine, dried over magnesium sulphate and then concentrated in vacuo. The crude product was purified on a chromatotron (silica, 6:4, petroleum ether/ ethyl acetate) producing 22 mg (0.086 mmol, 48%) of 2-(2-methyl-4-aminophenyl)-6-hydroxybenzo[ $\beta$ ]thiophene. H NMR (CD<sub>3</sub>OD) 7.54 (d, J = 8.6, 1H), 7.18 (d, J = 2.4 Hz, 1H), 7.17 (d, J = 8.6, 1H), 7.00 (s, 1H), 6.84 (dd, J = 8.6, 2.4 Hz, 1H), 6.64 (d, J = 2.4 Hz, 1H), 6.58 (dd, J = 8.6, 2.4 Hz), 2.37 (s, 3H).

#### Example 21

## 2-(2-methyl-3-nitrophenyl)-6-hydroxybenzo[ $\beta$ ]thiophene (17).

- (a) The cross-coupling of 432 mg (2.0 mmol) 2-bromo-6- nitrotoluene with 982 mg (3.0 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 95:5, petroleum ether/ ethyl acetate) producing 114 mg (0.38 mmol, 13%) of 2-(2-methyl-3-nitrophenyl)-6-methoxybenzo[β]thiophene.
- mmol) 2-(2-methyl-3deprotection of 200 mg (0.67)The (b) nitrophenyl)-6-methoxybenzo[β]thiophene (example (17a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 70:30, petroleum ether/ ethyl acetate) producing 101 mg (0.35 mmol, 53%) of 2-(2-methyl-3-nitrophenyl)-6-hydroxybenzo[β]thiophene. H NMR (CDCOCD<sub>3</sub>) 8.67 (s, 1H), 7.86 (dd, J = 8.0, 1.2 Hz, 1H), 7.76 (dd, J = 7.7, 1.2 Hz, 1H), 7.73 (d, J = 8.7Hz, 1H), 7.54 (m, 1H), 7.38 (d, J = 2.1 Hz, 1H), 7.36 (s, 1H), 7.00 (dd, J = 8.7, 2,1 Hz, 1H), 5.15 (s, 1H), 2.52 (s, 3H).

#### Example 22

2-(2-methyl-3-aminophenyl)-6-hydroxybenzo[β]thiophene (18).

350 mg (1.23 mmol) of 2-(2-methyl-3-nitrophenyl) -6-hydroxybenzo[ $\beta$ ]thiophene

(example (17(b)) was dissolved in 10 ml of ethanol and 1384 mg (6.1 mmol) of tin dichloride dihydrate was added. The mixture was heated to 70°C under a nitrogen atmosphere for 3 hours. Hydrochloric acid (1 M) was added and then the aqueous phase was extracted with ethyl acetate. The combined organic phases were washed with brine, dried over magnesium sulphate and then concentrated in vacuo. The crude product was purified on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) producing 27 mg (0.10 mmol, 8.1%) of 2-(2-methyl-3-aminophenyl)-6-hydroxybenzo[β]thiophene. <sup>1</sup>H NMR (CD<sub>3</sub>OD) 8.93 (s, 1H broad), 7.65 (d, J = 8.8, 1H), 7.33 (d, J = 2.5 Hz, 1H), 7.12 (s, 1H), 6.92-7.00 (m, 2H), 6.71-6.78 (m, 2H), 4.69 (s, 2H broad), 2.20 (s, 3H).

## Example 23

 $2-(2-methyl-3-bromo-5-hydroxyphenyl)-6-hydroxybenzo[<math>\beta$ ]thiophene (19).

- (a) The cross-coupling of 369 mg (1.3 mmol) 2,6-dibromo-4- methoxytoluene with 636 mg (1.95 mmol) of the product from  $\mathbf{1}(a)$  was accomplished by the procedure set forth in example  $\mathbf{1}(b)$ . The crude product was purified on a chromatotron (silica, 98:2, petroleum ether/ ethyl acetate) producing 220 mg (0.61 mmol, 46.6%) of 2-(2-methyl-3-bromo-5-methoxyphenyl)-6-methoxybenzo[ $\beta$ ]thiophene.
- mmol) 2-(2-methyl-3-bromo-5-70 mg (0.19)deprotection of (b) The methoxyphenyl)-6-methoxybenzo[ $\beta$ ]thiophene (example (19a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica. 8:2, petroleum ether/ ethyl acetate) producing 55 mg (0.16 mmol, 86%) of 2-(2-methyl-3-bromo-5- hydroxyphenyl)-6-hydroxybenzo[β]thiophene. 'H NMR (CDCOCD<sub>2</sub>) 8.66 (s, 1H), 7.69 (d, J = 8.4, 1H), 7.34 (d, J = 2.2 Hz, 1H), 7.23 (s, 1H), 7.15 (d, J = 2.5 Hz, 1H), 6.99 (d, J = 2.2 Hz, 1H), 7.00 (dd, J = 8.4, 2,2 Hz, 1H), 6.94 (d, J = 2.5 Hz, 1H), 2.38 (s, 3H).

## Example 24

## 2-(2-methyl-5-hydroxyphenyl)-6-hydroxybenzo[β]thiophene (20).

- (0.08)a) 30 mg mmol) 2-(2-methyl-3-bromo-5-methoxyphenyl) -6-methoxybenzo[β]thiophene (example (19a) was dissolved in 2 ml of tetrahydrofuran. The mixture was cooled to -70°C and butyllithium (0.12 mmol) was added to the reaction mixture. The reaction mixture was stirred for 2.5 hours at -70°C and then at room temperature overnight. The reaction mixture was quenched with aqueous ammonium chloride, extracted with ethyl acetate and dried over magnesium sulphate. This produced 30 mg of crude 2-(2-methyl-5-methoxyphenyl) -6-methoxybenzo[β]thiophene.
- b) The deprotection of 30 mg (0.10)mmol) 2-(2-methyl-5methoxyphenyl)-6-methoxybenzo[ $\beta$ ]thiophene (example (20a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on HPLC (reversed phase, C18, gradient, acetonitrile/water + 0.05 trifluoroacetic acid) producing 6.7 (0.026)mmol, 24%) of 2-(2-methyl-5-hydroxyphenyl) -6-hydroxybenzo[β]thiophene. H NMR (CD<sub>3</sub>COCD<sub>3</sub>) 8.55 (s, 1H), 8.29 (s, 1H), 7.67 (dd, J = 8.5, 2.2 Hz, 1H), 7.33 (t, 1H), 7.24 (d, J = 2.5, 1H), 7.13 (dd, J = 8.2, 2.0 Hz, 1H)1H), 6.92-6.99 (m, 2H), 6.76 (dt, 1H), 2.35 (d, J = 2.2 Hz, 3H).

## Example 25

2-phenyl-6-hydroxybenzo[β]thiophene (21).

The cross-coupling of 157 mg (1.0 mmol) bromobenzene with 491 mg (1.5 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was deprotected by the procedure set forth in example 1 (c). It was purified on a chromatotron (silica, 9:1, petroleum ether/ ethyl acetate) producing 81 mg (0.36 mmol, 36%) 2-phenyl-6-hydroxybenzo[β]thiophene. <sup>1</sup>H NMR (CD<sub>3</sub>COCD<sub>3</sub>) 8.65 (s 1H), 7.60-7.75 (m, 4H), 7.28-7.48 (m, 4H), 6.95 (dd, J = 8.5, 2.5 Hz, 1H).

Example 26

2-(4-hydroxyphenyl)-benzo[ $\beta$ ]thiophene (22).

- (a) The stannylation of 3 g (22.4 mmol) of benzo[ $\beta$ ]thiophene was accomplished by the procedure set forth in example 1(a). This produced 6.3 g (21.3 mmol) of 2-trimethylstannylbenzo[ $\beta$ ]thiophene.
- (b) The cross-coupling of 468 mg (2.0 mmol) 4-iodophenol with 889 mg (3.0 mmol) of the product from 22(a) was accomplished by the procedure set forth in example 1(b). The crude product was deprotected by the procedure set forth in example 1 (c) and then purified on a chromatotron (silica, 9:1, petroleum ether/ ethyl acetate) and recrystalised (petroleum ether/ ethyl acetate) producing 20 mg (0.09 mmol, 4%) of 2-(4-hydroxyphenyl)-benzo[β]thiophene. <sup>1</sup>H NMR (CD<sub>3</sub>COCD<sub>3</sub>) 8.70 (s 1H), 7.88 (m, 1H), 7.79 (m, 1H), 7.56-7.69 (m, 3H), 7.25-7.38 (m, 2H), 6.90-7.00 (m, 2H).

## Example 27

 $2-(2-trifluoromethyl-6-fluorophenyl)-6-hydroxybenzo[<math>\beta$ ]thiophene (23).

Produced in a parallell solution phase way. A mixture of 61 mg (0.25 mmol) 2-bromo-3-fluorobenzotrifluoride, (0.013)mmol) tetrakis 15 mg triphenylphosphinepalladium (0) and 20 mg (0.25 mmol) of cupric oxide in 1 ml of N,N-dimethylformamide was stirred at 100°C under nitrogen. After 5 minutes, 123 mg (0.38 mmol) of 2-trimethylstannyl-6-methoxybenzo[ $\beta$ ]thiophene (example 1(a)) in 2 ml of N,N-dimethylformamide was added all at once to the reaction mixture. The solution was heated to 100°C for 3 hours, concentrated on a speed-vac, dissolved in dichloromethane, filtered through a silica pad and then concentrated again. The product was dissolved in 1.5 ml of dichloromethane and 1 ml of boron trifluoride dimethylsulfide complex was added. The reaction mixture was stirred overnight in darkness, quenched with water and extracted with dichloromethane. The organic phase

was dried by passing it through sodium sulphate dryingtubes and then it was concentrated in a speed-vac. The crude product was purified on HPLC (silica, n-heptane + 0.5% acetic acid to ethyl acetate + 0.5% acetic acid as gradient eluent) producing 1.5 mg (0.005 mmol, 2%) of 2-(2-trifluoromethyl-6-fluorophenyl)-6-hydroxybenzo[ $\beta$ ]thiophene. <sup>1</sup>H NMR (CD<sub>3</sub>COCD<sub>3</sub>) 8.72 (s, 1H broad), 7.71-7.78 (m, 3H), 7.55-7.65 (m, 1H), 7.37 (d, J = 2.2. Hz, 1H), 7.29 (s, 1H), 6.99 (dd, J = 8.7, 2.2 Hz, 1H).

## Example 28

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## 6-(6-hydroxy-2-benzo[β]thienyl)-4,5-dimethylbenzo-2,1,3-thiadiazole (24).

The cross-coupling of 61 mg (0.25 mmol) 6-bromo-4,5-dimethylbenzo-2, 1,3-thiadiazole with 123 mg (0.38 mmol) of the product from **1**(a) and the subsequent deprotection was accomplished by the procedure set forth in example **23.** The crude product was purified on HPLC (silica, n-heptane + 0.5% acetic acid to ethyl acetate + 0.5% acetic acid as gradient eluent) producing 3.6 mg (0.012 mmol, 4.6%) of 6-(6-hydroxybenzo[β]thien-2-yl)-4,5-dimethylbenzo-2,1,3-thiadiazole. <sup>1</sup>H NMR (CD<sub>3</sub>COCD<sub>3</sub>) 7.92 (s 1H), 7.74 (d, J = 8.5, 1H), 7.38 (d, J = 2.2 Hz, 1H), 7.37 (s, 1H), 7.01 (dd, J = 8.5, 2.2 Hz, 1H), 2.76 (s, 3H), 2.50 (s, 3H).

#### Example 29

2-(4-methyl-3-thienyl)-6-hydroxybenzo[β]thiophene (25).

The cross-coupling of 44 mg (0.25 mmol) 3-bromo-4-methylthiophene with 123 mg (0.38 mmol) of the product from 1(a) and the subsequent deprotection was accomplished by the procedure set forth in example 23. The crude product was purified on HPLC (silica, n-heptane+ 0.5% acetic acid to ethyl acetate + 0.5% acetic acid as gradient eluent) producing 22 mg (0.09 mmol, 36%) 2-(4-methyl-3-thienyl)-6-hydroxybenzo[β]thiophene. <sup>1</sup>H NMR (CD<sub>3</sub>COCD<sub>3</sub>) 8.57 (s

1H), 7.66 (d, J = 8.4, 1H), 7.53 (d, J = 3.2 Hz, 1H), 7.35 (s, 1H), 7.32 (m, 1H),

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2-(3,4,5-trimethyl-2-thienyl)-6-hydroxybenzolβlthiophene (26).

The cross-coupling of 252 mg (01.0 mmol) 2-iodo-3,4,5-trimethylthiophene with 491 mg (1.5 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude 2-(3,4,5-trimethyl-2-thienyl)-6-methoxybenzo[β] thiophene was deprotected by the procedure set forth in example 1 (c) and then purified on a chromatotron (silica, 9:1, petroleum ether/ ethyl acetate) producing 180 mg (0.625 mmol, 63%) of 2-(3,4,5-trimethyl-2-thienyl)-6-hydroxybenzo[β] thiophene. <sup>1</sup> H NMR (CD<sub>3</sub>COCD<sub>3</sub>) 8.55 (s, 1H), 7.67 (d, J = 8.7 Hz, 1H), 7.32 (d, J = 2.2 Hz, 1H), 7.06 (d, J= 0.7 Hz, 1H), 6.95 (dd, J= 8.7, 2.2 Hz, 1H), 2.34 (s, 3H), 2.30 (s, 3H), 1.96 (s, 3H).

## Example 31

 $2-(5-(1,3-dimethyluracilyl))-6-hydroxybenzo[\beta] thiophene (27).$ 

- (a) The cross-coupling of 266 mg (1.0 mmol) 5-iodo-1,3-dimethyluracil with 491 mg (1.5 mmol) of the product from  $\mathbf{1}(a)$  was accomplished by the procedure set forth in example  $\mathbf{1}(b)$ . The crude product was purified on a chromatotron (silica, 40:1, dichloromethane/ ethyl acetate) producing 211 mg (0.625 mmol, 63%) of 2-(5-(1,3-dimethyluracilyl))-6-methoxybenzo[ $\beta$ ] thiophene.
- (b) The deprotection of 30 mg (0.10 mmol) of 2-(5-(1,3-dimethyluracilyl))-6-methoxybenzo[ $\beta$ ] thiophene (example (27a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatothron (silica, 9:1, petroleum ether/ ethyl acetate) producing 1.2 mg (0.004 mmol, 4.2%) of

 $2-(5-(1.3-\text{dimethyluracilyl}))-6-\text{hydroxybenzo}[\beta]$  thiophene <sup>1</sup> H NMR (CDCl<sub>3</sub>) 7.74 (s, 1H), 7.61 (d, J = 8.7 Hz, 1H), 7.54 (s, 1H), 7.10-7.30 (m, 1H), 7.13 (dd, J = 8.7, 2.3 Hz, 1H), 3.87 (s, 3H), 3.51 (s, 3H).

#### Example 32

# [2-(4-hydroxyphenyl)-6-hydroxybenzo[\beta] thien-3-yl][phenyl]methanone (28).

- (a) To 200 mg, (0.74 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser et al, WO 96/30361) and 110 mg (0.78 mmol) benzoyl chloride in dichloro methane (5 ml) was added 740 mg (5.6 mmol) aluminium chloride. The reaction mixture was stirred for 5 hours at room temperature. The reaction was quenched by the addition of ethyl acetate and 1 M hydrochloric acid. The organic layer was separated and the aqueous phase was extracted with ethyl acetate. The combined organic phases were dried over magnesium sulphate, filtered and concentrated. The crude product was purified on a chromatotron (silica, 95:5, petroleum ether/ethyl mmol, 47%) 131 m g (0.35)acetate) producing [2-(4-methoxyphenyl)-6-methoxybenzo[\beta] thien-3-yl]phenylmethanone as yellow crystals.  $^{1}$ H NMR (CDCl<sub>3</sub>) 7.72-7.80 (m, 2H) 7.59 (d, J = 8.9 Hz, 1H), 7.36-7.43 (m, 1H), 7.21-7.34 (m, 5H), 6.97 (dd, J = 8.9, 2.5 Hz, 2H) 6.72 (m, 1H), 3.88 (s, 3H), 3.72 (s, 3H).
- (b) 70 mg, (0.19 mmol) [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl] phenylmethanone (example 28a) was dissolved in dichloromethane (5 ml), put under nitrogen atmosphere and cooled to -5°C. To the stirred solution was added 0.56 ml (0.56 mmol) 1M BBr<sub>3</sub> dropwise. The reaction mixture was stirred for 1 hour at 5°C, poured into ice water and extracted with ethyl acetate. The organic phase was dried over magnesium sulphate, filtered and concentrated. The crude product was purified on a chromatotron (silica, 75:25 to 50:50, petroleum ether/ ethyl acetate as gradient eluent) producing 46 mg (0.13 mmol, 71%) of [2-(4-hydroxyphenyl) -6-hydroxybenzo[β] thien-3-yl]phenylmethanone as yellow crystals. MP 214-217°C,

<sup>1</sup>H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.74 (s, 1H), 8.64 (s, 1H), 7.70-7.77 (m, 2H), 7.20-7.54 (m, 7H), 6.96 (dd, J = 8.7, 2.4 Hz, 1H), 6.68-6.76 (m, 2H).

## Example 33

# [2-(4-hydroxyphenyl)-6-hydroxybenzo[\beta] thien-3-yl][2-naphthyl]methanone (29).

- (a) The acylation of 150 mg, (0.55 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[ $\beta$ ] thiophene (Hauser *et al*, WO 96/30361) with 111 mg (0.58 mmol) 2-naphthoyl chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 95:5, petroleum ether/ethyl acetate) producing 105 mg (0.25 mmol, 45%) of [2-(4-methoxyphenyl)-6-methoxybenzo[ $\beta$ ] thien-3-yl][2-naphthyl]methanone as yellow crystals. H nmr (CDCl<sub>3</sub>) 8.21 (s, 1H), 7.95 (dd, J = 8.7, 1.7 Hz, 1H), 7.71 (m, 3H), 7.31-7.61 (m, 6H), 6.96 (dd, J = 8.9, 2.5 Hz, 1H), 6.65 (m, 2H), 3.88 (s, 3H), 3.63 (s, 3H).
- (b) The deprotection of 70 mg (0.17 mmol) of [2-(4-methoxyphenyl)-6thien-3-yl][2-naphthyl]methanone (example **29**(a)) methoxybenzo[β] was accomplished by the procedure set forth in example 28 (b). The crude product was purified on a chromatotron (silica, 75:25 to 50:50, petroleum ether/ ethyl acetate as mmol. 72%) producing 47 m g (0.12)eluent) gradient [2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][2-naphthyl]methanone as yellow crystals. MP 229-232°C. H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.73 (s, 1H), 8.52 (s, 1H), 8.24 (s, 1H), 7.83-7.98 (m, 4H), 7.41-7.63 (m, 4H), 7.22-7.33 (m, 2H), 6.96 (dd, J=8.8, 2.2 Hz, 1H), 6.65 (m, 2H).

## Example 34

[2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-tert-butylphenyl] methanone (30).

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- (a) The acylation of 150 mg, (0.55 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser *et al*, WO 96/30361) with 115 mg (0.58 mmol) 4-tert-butylbenzoyl chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 95:5, petroleum ether/ethyl acetate) producing 125 mg (0.29 mmol, 52%) of [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-tert-butylphenyl]methanone as yellow crystals. H nmr (CDCl<sub>3</sub>) 7.64-7.73 (m, 2H), 7.55 (d, J = 8.9 Hz, 1H), 7.22-7.34 (m, 5H), 6.95 (dd, J = 8.9, 2.5 Hz, 1H), 6.72 (m, 2H), 3.87 (s, 3H), 3.71 (s, 3H), 1.22 (s, 9H).
- (b) The deprotection of 70 mg (0.17 mmol) 2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-tert-butylphenyl]methanone (example (30a)) was accomplished by the procedure set forth in example 28 (b). The crude product was purified on a chromatotron (silica, gradient 75:25 to 50:50, petroleum ether/ ethyl acetate) producing 30 mg (0.07 mmol, 46%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl] [4-tert-butylphenyl]methanone as yellow crystals. MP 197-200°C, <sup>1</sup>H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.69 (s, 1H), 8.60 (s, 1H), 7.63-7.70 (m, 2H), 7.35-7.46 (m, 4H), 7.21-7.28 (m, 2H), 6.94 (d, J = 8.8, 2.2 Hz, 1H), 6.72 (m, 2H), 1.28 (s, 9H).

## Example 35

# [2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ]thien-3-yl][4-methoxyphenyl]methanone (31).

(a) The acylation of 150 mg, (0.55 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[ $\beta$ ] thiophene (Hauser *et al*, WO 96/30361) with 99 mg (0.58 mmol) 4-methoxybenzoyl chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 95:5, petroleum ether/ethyl acetate) producing 112 mg (0.27 mmol, 50%) of [2-(4-methoxyphenyl)-6-methoxybenzo[ $\beta$ ] thien-3-yl][4-methoxyphenyl]methanone as yellow crystals.

(b) The deprotection of 70 mg (0.17 mmol) 2-(4-methoxyphenyl)-6-methoxybenzo[ $\beta$ ] thien-3-yl][4-methoxyphenyl]methanone(example (31a)) was accomplished by the procedure set forth in example 28 (b). The crude product was purified on a chromatotron (silica, 50:50, petroleum ether/ ethyl acetate) producing 40 mg (0.07 mmol. 63%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ]thien-3-yl] [4-methoxyphenyl]methanone as yellow crystals. H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.71 (s, 2H broad), 7.73 (m, 2H), 7.38-7.42 (m, 2H), 7.28(m, 2H), 6.94 (dd, J = 8.4, 2.4 Hz, 1H), 6.86 (m, 2H), 6.75 (m, 2H), 3.79 (s, 3H).

## Example 36

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[2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-carboxyphenyl]methanone (32).

- (a) The acylation of 506 mg, (1.87 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[ $\beta$ ] thiophene (Hauser *et al*, WO 96/30361) with 390 mg (1.97 mmol) terephthalic acid monomethyl ester chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 8:2 petroleum ether/ethyl acetate) producing 442 mg (1.02 mmol, 55%) of [2-(4-ethoxycarbonylphenyl] 6-methoxybenzo[ $\beta$ ] thien-3-yl] [4-methoxycarbonylphenyl]methanone.
- (b) The deprotection of 406 mg (0.94 mmol) [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-methoxycarbonylphenyl]methanone. (example (32a)) was accomplished by the procedure set forth in example 1 (c). The crude product was purified by recrystallisation (acetic acid/ dichloromethane/ methanol) producing 270 mg (0.69 mmol, 73%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-carboxyphenyl]methanone. H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.76 (s, 1H broad), 8.63 (s, 1H broad), 7.92-7.98 (m, 2H), 7.76-7.83 (m, 2H), 7.63 (d, J = 8.8 Hz, 1H), 7.41 (d, J = 2.5 Hz, 1H), 7.21 (m, 2H), 6.99 (dd, J = 8.8, 2.5 Hz, 1H), 6.69 (m, 2H).

Example 37

[2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ]thien-3-yl][4-methoxycarbonylphenyl]methanone (33).

[4-carboxyphenyl]methanone (example 32(b)) were dissolved in methanol and five drops of thionyl chloride were added. The reaction mixture was stirred at room temperature for 24 hours, quenched with water, extracted with ethyl acetate and dried over magnesium sulphate. The crude product was purified on a chromatothron (silica, 9:1 petroleum ether/ethyl acetate) producing 42 mg (0.1 mmol, 42%) of  $2 - (4 - h y d r o x y p h e n y 1) - 6 - h y d r o x y b e n z o [<math>\beta$ ] thien - 3 - y l] [4 - methoxycarbonylphenyl]methanone. H nmr (CD<sub>3</sub>OD) 8.76 (s, 1H broad), 7.82-7.88 (m, 2H), 7.66-7.72 (m, 2H), 7.61 (d, J = 8.9 Hz, 1H), 7.28 (d, J = 2.4 Hz, 1H), 7.08-7.14 (m, 2H), 6.90 (dd, J = 8.9, 2.4 Hz, 1H), 6.53-6.60 (m, 2H), 3.85 (s, 3H).

#### Example 38

[2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-ethoxycarbonylphenyl]methanone (34).

50 mg (0.12 mmol) [2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-carboxyphenyl]methanone (example 32(b)) were dissolved in ethanol and five drops of thionyl chloride were added. The reaction mixture was stirred at room temperature for 24 hours, quenched with water, extracted with ethyl acetate and dried over magnesium sulphate. The crude product was purified on a chromatothron (silica, 9:1 petroleum ether/ethyl acetate) producing 39 mg (0.1 mmol, 74%) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ]thien-3-yl][4-ethoxycarbonylphenyl]methanone. <sup>1</sup>H nmr (CD<sub>3</sub>OD) 8.72 (s, 2H broad), 7.87-7.94 (m, 2H), 7.76-7.82 (m, 2H), 7.62 (d, J = 8.8 Hz, 1H), 7.42 (d, J = 2.2 Hz, 1H), 7.17-7.24 (m, 2H), 6.99 (dd, J = 8.8, 2.2

Hz. 1H), 6.66-6.72 (m, 2H), 4.31 (q, 2H), 1.32 (t, 3H).

Example 39

[2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-cyanophenyl]methanone (35).

- (a) The acylation of 300 mg, (1.11 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser *et al*, WO 96/30361) with 193 mg (1.17 mmol) 4-cyanobenzoyl chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 8:2 petroleum ether/ethyl acetate) producing 206 mg (0.52 mmol, 46%) of [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-cyanophenyl]methanone.
- (b) The deprotection of 30 mg (0.075 mmol) [2-(4-methoxyphenyl)-6-methoxybenzo[ $\beta$ ] thien-3-yl][4-cyanophenyl]methanone (example (35a)) was accomplished by the procedure set forth in example 1 (c). The crude product was purified on a chromatotron (silica, 5:5 petroleum ether/ethyl acetate) producing 24 mg (0.06 mmol, 86%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-cyanophenyl]methanone. H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.77 (s, 1H broad), 8.73 (s, 1H broad), 7.78-7.85 (m. 2H), 7.65-7.73 (m. 3H), 7.43 (d, J = 2.2 Hz, 1H), 7.16 (m 2H), 7.02, (dd, J = 8.8, 2.2 Hz, 1H), 6.69 (m, 2H).

Example 40

[2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-(1H-tetrazol-5-yl) phenyl]methanone (36).

30 mg (0.08 mmol) [2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-cyanophenyl]methanone (example 35(b)) was dissolved in 1 ml of N, N-dimethylformamide and kept under nitrogen. To the reaction mixture was added 49

mg (0.08 mmol) sodium azide and 40 mg (0.08 mmol) ammonium chloride, then it was heated to reflux temperature for 2 hours. The *N*, *N*-dimethylformamide was removed in a speed-vac. The compound was deprotected by the procedure set forth in example 1 (c). The crude product was purified on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) producing 24 mg (0.06) mmol, 72%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-(1H-tetrazol-5-yl) phenyl]methanone. H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.80 (s, 1H), 8.65 (s, 1H), 8.00-8.12 (m, 2H), 7.86-7.92 (m, 2H), 7.62 (d, J = 8.8 Hz, 1H), 7.42 (d, J = 2.2 Hz, 1H), 7.18-7.28, (m, 2H), 7.00 (dd, J = 8.8, 2.2 Hz, 1H), 6.65-6.75 (m, 2H).

### Example 41

5-oxo-5-[2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ]thien-3-yl]pentanoic acid methyl ester (37).

- (a) The acylation of 200 mg, (0.74 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser *et al*, WO 96/30361) with 139 mg (0.78 mmol) methyl adipoyl chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 9:1 petroleum ether/ethyl acetate) producing 91 mg (0.22 mmol, 30%) of 5-oxo-5-[2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl]pentanoic acid methyl ester.
- (b) The deprotection of 80 mg (0.19 mmol) 5-oxo-5-[2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl]pentanoic acid methyl ester (example (37a)) was accomplished by the procedure set forth in example 1 (c). The crude product was purified on a chromatotron (silica, 98:2 chloroform/methanol + acetic acid) producing 38 mg (0.10 mmol, 52%) of 5-oxo-5-[2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl]pentanoic acid methyl ester. <sup>1</sup>H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.86 (s, 1H broad), 8.67 (s, 1H broad), 7.82 (d, J = 8.8 Hz, 1H), 7.28-7.40 (m, 3H), 6.95-7.05 (m 3H), 3.56 (s, 3H), 2.37-2.46 (m, 2H), 2.11-2.20 (m, 2H), 1.36-1.60 (m, 4H).

Example 42

5-oxo-5-[2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl]pentanoic acid (38).

25 mg (0.06 mmol) of 5-oxo-5-[2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl] pentanoic acid methyl ester (example 37(b) was dissolved in five ml of methanol and 0.5 ml of 1 M sodium hydroxide. The reaction mixture was stirred for one hour, neutralized, extracted with ethyl acetate and dried over magnesium sulphate. This produced 11 mg (0.03 mmol, 49%) of 5-oxo-5-[2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl]pentanoic acid. <sup>1</sup>H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 7.82 (d, J = 8.8 Hz, 1H), 7.28-7.40 (m, 3H), 6.90-7.05 (m 3H).

Example 43

[2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-propylphenyl]methanone (39).

- (a) The acylation of 200 mg, (0.74 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[ $\beta$ ] thiophene (Hauser *et al*, WO 96/30361) with 142 mg (1.17 mmol) 4-propylbenzoyl chloride was accomplished by the procedure set forth in example 28(a). The crude product was purified on a chromatotron (silica, 9:1 petroleum ether/ethyl acetate) producing 128 mg (0.52 mmol, 42%) of [2-(4-methoxyphenyl)-6-methoxybenzo[ $\beta$ ] thien-3-yl][4-isopropylphenyl]methanone.
- (b) The deprotection of 100 mg (0.24 mmol) [2-(4-methoxyphenyl)-6-methoxybenzo [β]thien-3-yl][4-isopropylphenyl]methanone.

(example (39a)) was accomplished by the procedure set forth in example 1 (c). The crude product was purified on a chromatotron (silica, 5:5 petroleum ether/ethyl acetate) producing 28 mg (0.07 mmol, 30%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo [β]thien-3-yl][4-propylphenyl]methanone. H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.71 (s, 1H), 8.62 (s, 1H), 7.62-7.70 (m, 2H), 7.45 (d, J = 8.8 Hz, 1H), 7.39 (d, J = 2.2 Hz, 1H), 7.21-7.28

(m 2H), 7.14-7.20 (m, 2H), 6.94, (dd, J = 8.8, 2.2 Hz, 1H), 6.68-6.75 (m, 2H), 2.55 (t, 2H), 1.58 (m, 2H), 0.88 (t, 3H).

#### Example 44

[2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-iodophenyl]methanone (40).

- a) The acylation of 200 mg, (0.74 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[ $\beta$ ] thiophene (Hauser *et al*, WO 96/30361) with 207 mg (0.77 mmol) 4-iodobenzoyl chloride was accomplished by the procedure set forth in example 28(a). The crude product was purified on a chromatotron (silica, 9:1 petroleum ether/ethyl acetate) producing 258 mg (0.52 mmol, 70%) of [2-(4-methoxyphenyl)-6-methoxybenzo[ $\beta$ ] thien-3-yl][4-iodophenyl]methanone.
- [β]thien-3-yl][4-iodophenyl]methanone.

  (example (40)) was accomplished by the procedure set forth in example 1 (c). The crude product was purified on a chromatotron (silica, 5:5 petroleum ether/ethyl acetate) producing 43 mg (0.09 mmol, 45%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4-iodophenyl]methanone. <sup>1</sup>H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.71 (s, 2H, broad), 8.62 (s, 1H), 7.69-7.78 (m, 2H), 7.54 (d, J = 8.8 Hz, 1H), 7.45-7.50 (m, 2H), 7.40 (d, J = 2.2 Hz, 1H), 7.17-7.24 (m 2H), 6.96, (dd, J = 8.8, 2.2 Hz, 1H),

(b) The deprotection of 100 mg (0.20 mmol) [2-(4-methoxyphenyl)-6-methoxybenzo

## Example 45

6.68-6.75 (m, 2H).

2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-acetylphenyl]methanone (41).

(a) A mixture of 246 mg (0.75 mmol) of hexamethylditin, 250 mg (0.50 mmol) of

[2-(4-methoxyphenyl)-6-methoxybenzo[β]thien-3-yl][4-iodophenyl] methanone. (example (39a)), 6 mg (0.005 mmol)) tetrakis triphenylphosphinepalladium (0) and 20 ml toluene was heated under reflux in a nitrogen atmosphere for 20 h. The reaction mixture was concentrated, dissolved in diethylether, washed with water twice, dried over magnesium sulphate, filtered and concentrated. This yielded 241 mg (0.45 mmol, 90%) of the desired [2-(4-methoxyphenyl)-6-methoxybenzo[β]thien-3-yl][4-trimethylstannylphenyl]methanone.

(b) 100 mg (0.19 mmol) of [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-trimethylstannylphenyl]methanone (example 41(a)) and 15 mg (0.19 mmol) of acetyl chloride was dissolved in 5 ml of toluene. To the reaction mixture was added 4.6 mg (0.0044 mmol) of tris(dibenzylideneacetone)palladium(0)\*chloroform. The reaction mixture was then heated under a nitrogen atmosphere at 70⑤ C 20 hours, filtered, extracted with ethyl acetate, washed with saturated sodium bicarbonate and dried over magnesium sulphate. The deprotection of the crude [2-(4-methoxyphenyl)-6-methoxybenzo[β]thien-3-yl][4-acetylphenyl]methanone was accomplished by the procedure set forth in example 1 (c). The product was purified on a chromatotron (silica, 5:5 petroleum ether/ethyl acetate) producing 61 mg (0.16 mmol, 82%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-acetylphenyl]methanone. <sup>1</sup>H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 7.85-7.92 (m, 2H), 7.76-7.83 (m, 2H), 7.59 (d, J = 8.8 Hz, 1H), 7.41 (d, J = 2.2 Hz, 1H), 7.17-7.24 (m 2H), 6.98, (dd, J = 8.8, 2.2 Hz, 1H), 6.66-6.73 (m, 2H), 2.54 (s, 3H).

## Example 46

 $2\text{-}(4\text{-hydroxyphenyl})\text{-}6\text{-hydroxybenzo}[\beta] \ thien\text{-}3\text{-yl}][4\text{-propionylphenyl}] methan one \\ (42).$ 

200 mg (0.38 mmol) of [2-(4-methoxyphenyl)-6-methoxybenzo[ $\beta$ ] thien-3-yl][4-trimethylstannylphenyl]methanone (example 41(a)) and 34 mg (0.38 mmol) of propionyl chloride was dissolved in 10 ml of toluene. To the reaction mixture was

added 9.2 mg (0.0088 mmol) of tris(dibenzylideneacetone)palladium(0)\*chloroform. The reaction mixture was then heated under a nitrogen atmosphere at 70°C for 20 hours, filtered, extracted with ethyl acetate, washed with saturated sodium bicarbonate and dried over magnesium sulphate. The deprotection of the crude [2-(4-methoxyphenyl)-6-methoxybenzo[β]thien-3-yl][4-propionylphenyl]methanone was accomplished by the procedure set forth in example 1 (c). The crude product was purified on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) producing 9 mg (0.02 mmol, 6%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4-propionylphenyl]methanone. H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.72 (s, 1H), 8.61 (s, 1H), 7.85-7.92 (m, 2H), 7.76-7.83 (m, 2H), 7.59 (d, J = 8.8 Hz, 1H), 7.41 (d, J = 2.2 Hz, 1H), 7.17-7.24 (m 2H), 6.98, (dd, J = 8.8, 2.2 Hz, 1H), 6.66-6.73 (m, 2H), 2.99 (q, 2H), 1.08 (t. 3H).

## Example 47

2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-buturylphenyl]methanone (43).

100 mg (0.19 mmol) of [2-(4-methoxyphenyl)-6-methoxybenzo[β]thien-3-yl][4-trimethylstannylphenyl]methanone (example 41(a)) and 22 mg (0.20 mmol) of buturyl chloride was dissolved in 5 ml of toluene. To the reaction mixture was added 4.6 mg (0.0044 mmol) of tris(dibenzylideneacetone)palladium(0)\*chloroform. The reaction mixture was then heated under a nitrogen atmosphere at 70°C for 20 hours, filtered, extracted with ethyl acetate, washed with saturated sodium bicarbonate and dried over magnesium sulphate. The crude product was purified on a chromatotron (silica, 9:1 petroleum ether/ethyl acetate). The deprotection of the crude [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-buturylphenyl]methanone was accomplished by the procedure set forth in example 1 (c). The product was purified on a chromatotron (silica, 9:1 petroleum ether/ethyl acetate) producing 17 mg (0.04 mmol, 22%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4-buturylphenyl]methanone. 

1 mmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.72 (s, 1H), 8.61 (s, 1H), 7.85-7.92 (m, 2H), 7.76-7.83 (m, 2H),

7.60 (d, J = 8.8 Hz, 1H), 7.42 (d, J = 2.2 Hz, 1H), 7.17-7.24 (m 2H), 6.99, (dd, J = 8.8, 2.2 Hz, 1H), 6.66-6.73 (m, 2H), 2.96 (q, 2H), 1.67 (m, 2H), 1.08 (t. 3H).

Example 48

WO 98/56812

[2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ]thien-3-yl][4-ethylthiocarbonylphenyl]-methanone (44).

mg (0.12 mmol) [2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4-carboxyphenyl]methanone (example 32(b)) were dissolved in ethanthiol and five drops of thionyl chloride were added. The reaction mixture was stirred at room temperature for 24 hours in a nitrogen atmosphere, quenched with water, extracted with ethyl acetate and dried over magnesium sulphate. The crude product was purified on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) producing 26 mg (0.06 mmol, 54%) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-ethylthiocarbonylphenyl]methanone. H nmr (CD<sub>3</sub>OD) 8.72 (s, 1H broad), 8.60 (s, 1H), 7.89-7.98 (m, 2H), 7.75-7.84 (m, 2H), 7.61 (d, J = 8.8 Hz, 1H), 7.42 (d, J = 2.5 Hz, 1H), 7.17-7.24 (m, 2H), 6.99 (dd, J = 8.8, 2.5 Hz, 1H), 6.66-6.72 (m, 2H), 2.89 (q, 2H), 1.32 (t, 3H).

Example 49

2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ khien-3-yl][4-hydroxyphenyl]methanone (45)

The deprotection of 2-(4-methoxyphenyl)-6-methoxybenzo[ $\beta$ ]thien-3-yl][4-methoxyphenyl]methanone (example (31a)) as described in example 31(b) produced after purification 2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ]thien-3-yl][4- hydroxyphenyl]methanone as a byproduct. H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.60-9.00 (s, 3H broad), 7.62-7.72 (m, 2H), 7.36-7.40 (m, 2H), 7.22-7.28 (m, 2H), 6.92 (dd, J = 8.6, 2.4 Hz, 1H), 6.68-6.80 (m, 4H).

Example 50

# 2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-methylamino carbonyl-phenyl]methanone (46)

2-(4-methoxyphenyl)-6-methoxybenzo[\beta] thien-3-yl][4-methoxycarbonylphenyl]methanone (example 32(b)) was deprotected to 2-(4-methoxyphenyl)-6-methoxybenzo[\beta] thien-3-yl][4-carboxyphenyl]methanone by dissolving in ethanol and stirring with 1M sodium hydroxide for 4 hours. The ethanol was evaporated and the aqueous phase was extracted with ethylacetate, dried over magnesium sulphate and evaporated. The following reaction was run in a parallell solution phase way. 20 mg (0.048 mmol) of 2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-carboxyphenyl]methanone was mixed in sequential order with 30 mg (0.058 mmol) of benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate (PyBOP), 3.6 mg (0.024 mmol) of N-hydroxybenzotriazole\*H<sub>2</sub>O (HOBt), 2.5 ml of N,N-dimethylformylamide, 12.4 mg (0.096 mmol) of N,N-diisopropylethylamine and 2.23 mg (0.096 mmol) of methylamine hydrochloride in a nitrogen atmosphere at room-temperature for 3 days. The reaction was diluted with ethyl acetate. The organic phase was washed with 10% citric acid, dried by passing through a 3 ml extube. Varian Chem. Elut, and concentrated on a speed-vac. The deprotection of 2-(4-methoxyphenyl)--6-methoxybenzo[β] thien-3-yl][4-methylaminocarbonylphenyl]methanone as described in example 1(c) produced after purification on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) 6 mg (0.015 mmol, 31%) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-methylaminophenyl]methanone. 'H nmr (CD<sub>2</sub>COCD<sub>3</sub>) 7.70-7.85 (m, 4H), 7.55 (d, J = 8.8, 1H), 7.41 (d, J = 2.2, 1H), 7.19-7.25 (m, 2H), 6.99 (d, J = 8.8, 2.2 Hz, 1H), 6.66-6.74 (m, 2H).

## Example 51

2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-isobutvlaminocarbonylphenyl]methanone (47)

This reaction was run in a parallell solution phase way by the procedure set forth in example 46, using isobutylamine hydrochloride (5.24 mg (0.096 mmmol)) instead of methylamine. The crude product was purified on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) producing 1.2 mg (0.0027 mmol, 5.6 %) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl][4-isobutylaminophenyl]-methanone. <sup>1</sup>H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 7.72-7.92 (m, 4H), 7.51 (d, J = 8.8, 1H), 7.42 (d, J = 2.2 Hz, 1H), 7.18-7.26 (m, 2H), 6.97 (dd, J = 8.8, 2.2 Hz, 1H), 6.66-6.76 (m, 2H).

Example 52

2-(4-hydroxyphenyl)-6-hydroxybenzo[ $\beta$ ] thien-3-yl]-[4-benzylaminocarbonylphenyl]methanone (48)

This reaction was run in a parallell solution phase way by the procedure set forth in example 46, using benzylamine hydrochloride (7.68 mg (0.096 mmol) instead of methylamine. The crude product was purified on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) producing 1.7 mg (0.0035 mmol, 7.4 %) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-bensylaminophenyl]-methanone. <sup>1</sup>H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.33 (s, broad), 7.85-7.91 (m, 2H), 7.75-7.82 (m, 2H), 7.53 (d, J = 8.8 Hz, 1H), 7.42 (d, J = 2.2 Hz, 1H), 7.18-7.36 (m, 7H), 6.98 (dd, J = 8.8, 2.2 Hz, 1H), 6.68-6.74 (m, 2H).

Example 53

15 mg (0.040 mmol) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-carboxyphenyl]methanone (example 32(b)) was mixed in sequential order with 40 mg (0.077 mmol) of benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluoro-phosphate (PyBOP), 4.9 mg (0.032 mmol) of N-hydroxybenzotriazole\*H<sub>2</sub>O (HOBt),

3.0 ml of *N*,*N*-dimethylformylamide, 16.5 mg (0.128 mmol) of N,N-diisopropylethylamine and 0.015 g (0.096 mmol) of L-serine methylester hydrochloride in a nitrogen atmosphere at room-temperature for 3 days. The reaction was diluted with ethyl acetate. The organic phase was washed with 1M hydrochloric acid and brine. Then dried over magnesium sulphate and evaporated to dryness. Purification on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) produced 7.4 mg (0.015 mmol, 38%) of 49. <sup>1</sup>H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 7.78-7.92 (m, 4H), 7.55 (d, J = 8.8, 1H), 7.41 (d, J = 2.2, 1H), 7.19-7.28 (m, 2H), 6.98 (dd, J = 8.8, 2.2 Hz, 1H), 6.66-6.74 (m, 2H), 4.69 (m, 1H), 3.95 (m, 2H), 3.69 (s, 3H).

#### Example 54

15 mg (0.040 mmol) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-carboxyphenyl]methanone (example 32(b)) was mixed in sequential order with 40 mg (0.077 mmol) of benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluoro-phosphate (PyBOP), 4.9 mg (0.032 mmol) of N-hydroxybenzotriazole\*H<sub>2</sub>O (HOBt), 3.0 ml of N,N-dimethylformylamide, 16.5 mg (0.128 mmol) of N,N-diisopropylethylamine and 0.013 g (0.096 mmol) of L-alanine methylester hydrochloride in a nitrogen atmosphere at room-temperature for 3 days. The reaction was diluted with ethyl acetate. The organic phase was washed with 1M hydrochloric acid and brine. Then dried over magnesium sulphate and evaporated to dryness. Purification on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) produced 17.4 mg (0.037 mmol, 91%) of 50. <sup>1</sup>H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.12 (s, 1H broad), 8.10 (s, 1H broad), 7.75-7.89 (m, 4H), 7.53 (d, J = 8.8, 1H), 7.41 (d, J = 2.2, 1H), 7.17-7.23 (m, 2H), 6.98 (dd, J = 8.8, 2.2 Hz, 1H), 6.69-6.74 (m, 2H), 4.59 (m, 1H), 3.66 (s, 3H), 1.45 (d, 3H).

#### Example 55

15 mg (0.040 mmol) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-carboxyphenyl]methanone (example 32(b)) was mixed in sequential order with 40 mg

(0.077 mmol) of benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluoro-phosphate (PyBOP), 4.9 mg (0.032 mmol) of N-hydroxybenzotriazole\*H<sub>2</sub>O (HOBt), 3.0 ml of N.N-dimethylformylamide, 16.5 mg (0.128 mmol) of N,N-diisopropylethylamine and 0.021 g (0.096 mmol) of L-phenylalanine methylester hydrochloride in a nitrogen atmosphere at room-temperature for 3 days. The reaction was diluted with ethyl acetate. The organic phase was washed with 1M hydrochloric acid and brine. Then dried over magnesium sulphate and evaporated to dryness. Purification on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) produced 10.9 mg (0.020 mmol, 51%) of 51. <sup>1</sup>H nmr (CD<sub>3</sub>COCD<sub>3</sub>) 8.01 (s, 1H broad), 7.98 (s, 1H broad), 7.75 (s, 4H), 7.53 (d, J = 8.8, 1H), 7.41 (d, J = 2.2, 1H), 7.15-7.31 (m, 7H), 6.98 (dd, J = 8.8, 2.2 Hz, 1H), 6.69-6.74 (m, 2H), 4.82 (m, 1H), 3.65 (s, 3H).

The biological character of the compounds prepared in accordance with Examples 1 to 26 and 28 to 40 inclusive and also, for comparison purposes estradiol was measured in a radioligand displacement assay. The affinity for ER $\alpha$  and ER $\beta$  was measured as an IC<sub>50</sub>, the concentration of ligand necessary to displace 50% of tritated 17- $\beta$ -estradiol from either hER $\alpha$  (human estrogen receptor  $\alpha$ ) or hER $\beta$  (human estrogen receptor  $\beta$ ) respectively. In this assay, it was found that the IC<sub>50</sub>'s of compounds varied from 2.0 nM to 20 $\mu$ M for ER $\alpha$  and from 2.0 nM to 12  $\mu$ M for ER $\beta$ . The ER $\alpha$ /ER $\beta$  selectivity ratio varied from 0.2 to 23.

## Experimental description of ER binding assay

Affinity for the ER (by displacement of <sup>3</sup>[H]-estradiol) ws measured using the scintistrip assay<sup>1</sup>. Human estrogen receptors (hER) alpha and beta were extracted from the nuclei from SF9-cells infected with a recombinant baculovirus transfer vector containing the cloned hER genes.<sup>2</sup> The concentration of hER's in the extract was measured as specific <sup>3</sup>[H]-E2 binding with the G25-assay.<sup>3</sup>

- 1) Haggblad, J., Carlsson, B., Kivelä, P., Siitari, H., (1995) Biotechniques 18, 146-151.
- 2) Barkhem, T., Carlsson, B., Simons, J., Moller, B., Berkenstam, A., Gustafsson

- J.A.G., Nilsson, S. (1991) J. Steroid Biochem. Molec. Biol. 38, 667-75.
- 3) Salononsson, M., Carlsson, B., Haggblad, J., (1994) J. Steroid Biochem. Molec. Biol. 50, 313-318.

### **CLAIMS**

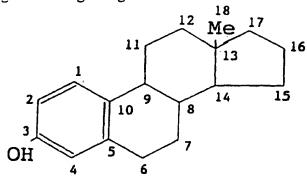
- 1. A crystal comprising at least a portion of the ERα ligand binding domain.
- 2. A crystal according to claim 1 comprising at least 200 amino acids of ERα.
- 3. A crystal according to claim 1 or claim 2 comprising at least 250 amino acids of  $ER\alpha$ .
- 4. A crystal according to claim 1,2 or 3 comprising entire ERa.
- 5. A crystal according to any preceding claim produced using a sequence including helix  $H_{\rm to}$  of  $ER\alpha$ .
- 6. A crystal according to any one of claims 1 to 5 usable in X-ray crystallography techniques.
- 7. A crystal according to any one of claims 1 to 6 including a ligand bound to  $ER\alpha$  or a portion thereof.
- 8. A crystal according to claim 7 in which the ligand is estradiol, raloxifene, or any other ligand that binds with high affinity ( $<10\mu M$ ) to ER $\alpha$ .
- 9. A crystal of ERα LBD according to any preceding claim belonging to the space group P2, and having the unit cell dimensions a=61.48Å, b=115.16Å, c=137.38Å.
- 10. A crystal of ER $\alpha$  LBD according to any preceding claim belonging to the space group P2 and having the unit cell dimensions a=104.53Å b=53.68Å c=102.71Å and  $\beta$ =116.79°.
- 11. A crystal of ERa LBD according to any one of claims 1 to 9 belonging to the

space group C2 and having the unit cell dimensions a=89.91Å b=75.09Å c=87.50Å and  $\beta$ =103.01°.

- 12. A crystal of ERα LBD according to any one of claims 1 to 9 belonging to the space group C222<sub>1</sub> and having the unit cell dimensions a=65.47Å b=95.99Å c=164.14Å.
- 13. A method for designing ligands which will bind to an estrogen receptor, the method comprising determining amino acid or acids of the ligand binding domain of the estrogen receptor which interact with a binding ligand, and selecting a ligand which is likely to bind to the receptor according to the structure of the potential ligand.
- 14. A method according to claim 13 in which interaction with ER $\alpha$  and ER $\beta$  are separately determined whereby ER-form selective ligands can be selected.
- 15. A method according to claim 13 or 14, in which for ERα selective ligands the design of the potential ligand uses a crystal according to any one of claims 1 to 12.
- 16. Ligands for estrogen receptors designed using a method according to claim 13, 14 or 15.
- 17. Ligands designed according to a method according to claim 14 which are specific for ER $\alpha$  or ER $\beta$ .
- 18. Ligands binding to at least the LBD of an ER with an affinity of between 20 pmol and 200 nM.
- 19. Ligands binding reversibly to at least the LBD of an ER.
- 20. A method of inhibiting estadiol activity in an animal, the method comprising

administering to the animal a ligand according to claim 19 or claim 20.

- 21. A method of inhibiting estradiol activity according to claim 20 comprising administering a ligand according to claim 18 or claim 19.
- 22. A pharmaceutical compound comprising a ligand according to any one of claims 16 to 19.
- 23. An estrogen agonist, an estrogen antagonist, a partial estrogen agonist, or a partial estrogen antagonist designed using a method according to claim 13, 14 or 15.
- 24. An ER $\alpha$  selective ligand having a structural group larger than methyl capable of fitting into the  $\beta$  cavity of the ER $\alpha$ .
- 25. An ERa selective ligand having the general formula Z



and having hydrophobic substituents at one or more of the  $8\beta$ ,15 $\beta$  or 18 positions.

- 26. An ER $\beta$  selective ligand having the formula Z of claim 25 and having hydrophobic substituents at one or more of the  $9\alpha$  or  $12\alpha$  positions.
- 27. An ERα selective ligand according to claim 25 or ERβ selective ligand according to claim 26 in which the hydrophobic substituent is selected from methyl groups, ethyl groups, iso-propyl groups, chlorine, bromine or iodine.
- 28. An ER $\alpha$  or ER $\beta$  selective ligand, in which the ligand is a 2'-,3'-.5'- and/or 6'-

substituted 2-aryl benzothiophene.

- 29. An ER $\alpha$  or ER $\beta$  selective ligand according to claim 28, which is substituted at one or more of the 2',3', 5' and 6' positions.
- 30. An ER $\alpha$  selective ligand according to claim 28, in which the substituted 2-aryl benzothiophene fills the  $\alpha$  and  $\beta$ -face cavities of the ER.
- 31. An ER $\alpha$  selective ligand, which is a 2-aryl benzotheiphene with a small hydrophobic substituent at one or more of the 2',3',5' and 6' positions.
- 32. An ER ligand capable of filling the hydrophobic cavity of ER-α.
- 33. A ligand according to claim 32 which has a hydrophobic substituent on the ethoxyphenyl sidechain to the piperidinyl nitrogen atom of raloxifene.
- 34. A ligand according to claim 31 or 32 in which the ligand has a hydrophobic sustituent selected from linear alkyl groups, perfluoroalkyl groups (-CH<sub>3</sub> to -CH<sub>10</sub>H<sub>21</sub>, -CF<sub>3</sub> to -C<sub>10</sub>F<sub>21</sub>), benzyl-(CH<sub>2</sub>Ph), benzyl-(methylene cyclohexyl groups).
- 35. An ER ligand having a structure capable of interacting with Glu-353 of ER $\alpha$  or with Glu-262 of ER $\beta$ .
- 36. An ER ligand having a structure capable of interacting with Arg-394 of ER $\alpha$  or with Arg-303 or ER $\beta$ .
- 37. An ER ligand having a structure capable of interacting with residue His-524 of  $ER\alpha$  or with His-432 of  $ER\beta$ .
- 38. An ER ligand having a structure capable of interacting with Met-421 or Leu-384 of ER $\alpha$  or with Ile-330 Met-293 of ER $\beta$ .

- 39. An ER $\alpha$  selective ligand having a structure capable of interacting with Met-421 and/or Leu-384 of ER $\alpha$ .
- 40. An ER $\beta$  selective ligand having a structure capable of interaction with Ile-330 and/or Met-293 of ER $\beta$ .
- 41. An ER $\beta$  selective ligand according to claim 40 in which substitutions larger than a methyl group are provided at the  $\alpha$  14,16 or 17 positions of the steroid nucleus.
- 42. An ER ligand having a structure capable of interacting with Leu-384 of ER $\alpha$  or Met-293 of ER $\beta$ .
- 43. An ERα selective ligand capable of interacting with Leu-384 of ERα.
- 44. An ERβ selective ligand capable of interacting with Met-293 of ERβ.
- 45. An ERβ selective ligand according to claim 40 further provided with substituents at the 2° or 3° positions of the 2-aryl benzothiophene nucleus.
- 46. An ER $\beta$  selective ligand having a substituent larger than a methyl group at the R<sub>2</sub>' position of a 6.3'-dihydroxybenzothiophene.
- 47. An ER $\alpha$  selective ligand having a substituent larger than a methyl group at either the R<sub>2</sub>' and/or R<sub>3</sub>' position of a 6,5'-dihydroxybenzothiophene.
- 48. A ligand selective for either ER $\alpha$  or ER $\beta$  in which the ligand comprises a position-6 substituent from the benzothiophene nucleus or position-3 substituent from the estradiol nucleus arranged to selectively bind to either the amino acid Ile-326 of ER $\alpha$  or Asn-236 of ER $\beta$ .
- 49. A ligand selective for either ERα or ERβ in which the ligand comprises a

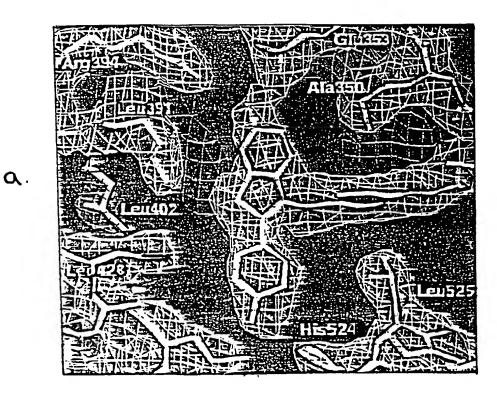
position-6 substituent from the benzothiophene nucleus or position-3 substituent from the estradiol nucleus arranged to selectively bind to either the amino acid Phe-445 of  $ER\alpha$  or Tyr-354 of  $ER\beta$ .

- 50. An ER $\alpha$  selective ligand having a structure capable of simultaneously interacting with Glu-323 and Phe-445 of ER $\alpha$  in preference to Glu-262 and Tyr-354 of ER $\beta$ .
- 51. An ER ligand having a structure arranged to promote binding with Helix H12 of the ER structure.
- 52. A crystal according to any of claims 1 to 12, having a resolution determined by X-ray crystallography less than 3.5Å.
- 53. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a crystal according to any one of claims 1 to 12 or a homologue of said crystal.
- 54. A method for evaluating the ability of a chemical entity to associate with an estrogen receptor, the method comprising the steps of:
- a) employing computational means to perform a fitting operation between the chemical entity and a binding site of the receptor; and
- b) analysing the results of the fitting operation to predict the association between the chemical entity and the binding site.
- 55. A crystallized molecule or molecular complex comprising a binding pocket defined by the structure coordinates of human ER-α ligand binding domain amino acid residues MET343, LEU346, THR347. LEU349, ALA350, ASP351, GLU353, LEU354, TRP383, LEU384, LEU387, MET388, LEU391, ARG394, PHE404, MET421, ILE424,

- PHE425, LEU428, GLY521, HIS524, LEU525 or a homologue of said molecular or molecular complex, wherein said homologue has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
- 56. A homology model comprising a binding pocket defined by the structure coordinates of human ER-β ligand binding domain amino acid residues MET343, LEU346. THR347. LEU349, ALA350, ASP351, GLU353, LEU354, TRP383, MET384. LEU387. MET388, LEU388, LEU391, ARG394, PHE404, ILE421, ILE424, PHE425, LEU428. GLY521, HIS524, LEU525.
- 57. A crystallized molecule or molecular complex comprising a binding pocket defined by the structure coordinates of rat ER-α ligand binding domain amino acid residues MET252, LEU255, THR256, LEU258, ALA259, ASP260, GLU262, LEU263, TRP292, LEU293, LEU296, MET297, LEU300, ARG303, PHE313, ILE330, IL333, PHE334, LEU337, GLY429, HIS423, LEU433 or a homologue of said molecule or molecular complex, wherein said homologue has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
- 58. A homology model comprising a binding pocket defined by the structure coordinates of rat ER-β ligand binding domain amino acid residues MET252, LEU255. THR256. LEU258, ALA259, ASP260, GLU262, LEU263, TRP292, MET293, LEU296, MET297, LEU300, ARG303, PHE313, ILE330, ILE333, PHE334, LEU337, GLY429, HIS432, LEU433.
- 59. A method of agonising or antagonising ER $\alpha$  or ER $\beta$ , the method comprising administering to a mammal a compound, other than raloxifene, that fits spatially into the binding pocket of ER $\beta$ .
- 60. A method according to claim 59 in which the compounds has at least one of the following:
  - a group capable of functioning as a hydrogen bond donor to HIS432;

- b) A group that functions as a hydrogen bond acceptor and donor to Arg-394 and Glu-353 of ERα or Arg-303 and Glu-262 of ERβ;
- c) a group capable of forming a hydrophobic contact with at least one of Met-252, Leu-255, Leu-258, Ala-259, Leu-263, Trp-292, Met-293, Leu-296, Met-297, Leu-300, Phe-313, Ile-330, Ile-333, Phe-334, Leu-337, Leu-433 of ERβ, or Met-343, Leu-346, Leu-349, Ala-350, Leu-354, Trp-383, Leu-384, Leu-387, Met-388, Leu-391, Phe-404, Met-421, Ile-424, Phe-425, Leu-428, Leu-525, of ERα.
- 61. A method of antagonising ER $\beta$  according to claim 59 or 60 in which the compound has a group that can form either a hydrogen bond or a salt bridge to ASP260.
- 62. A method of antagonising ER $\alpha$  according to claim 59 or 60 in which the compound has a group that can form either a hydrogen bond or a salt bridge to Asp-351.
- 63. An ER ligand in accordance with any one of the Examples 5 to 55.

### FIGURE 1



Ь.

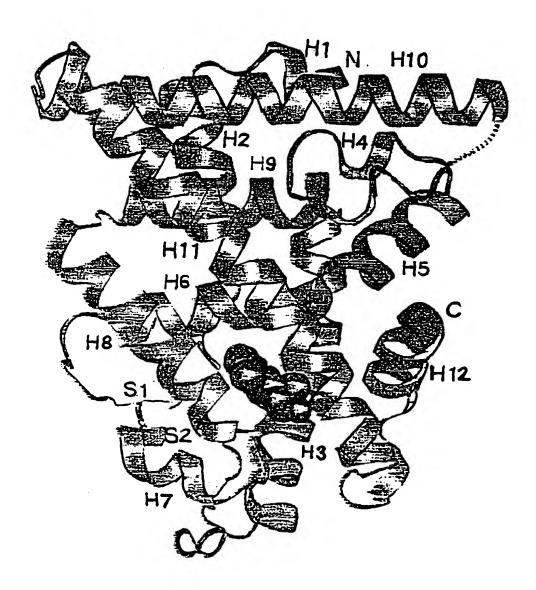
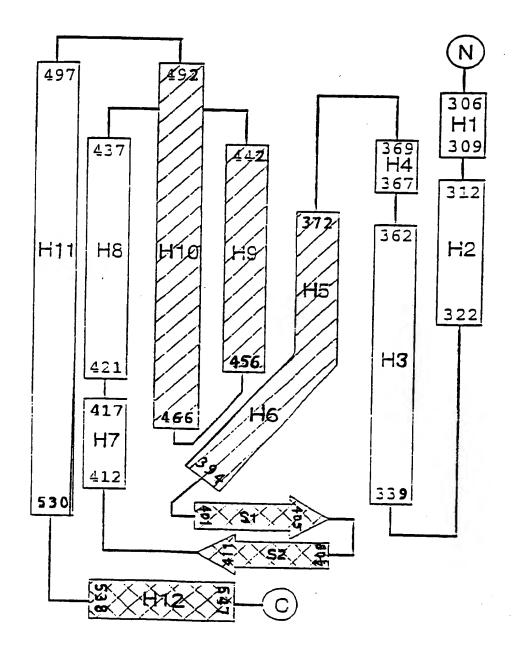
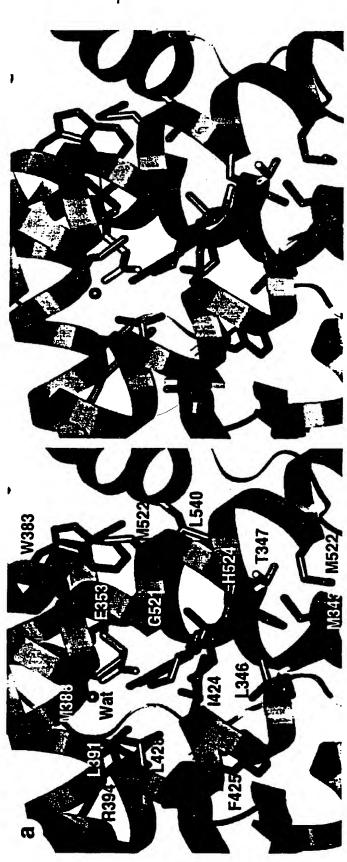


FIGURE 2a

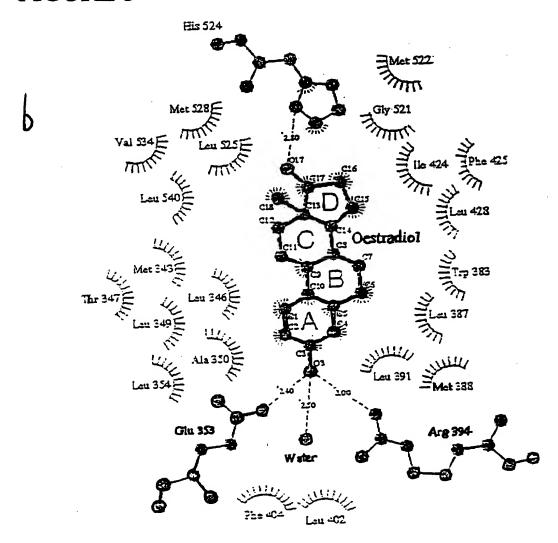
## FIGURE 2b

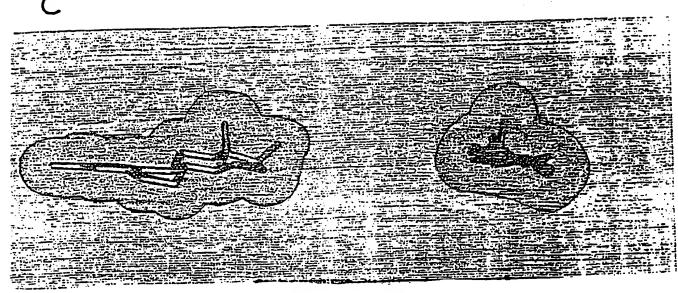




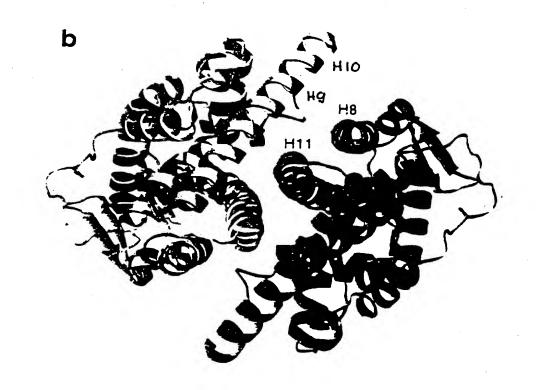


## FIGURE 3

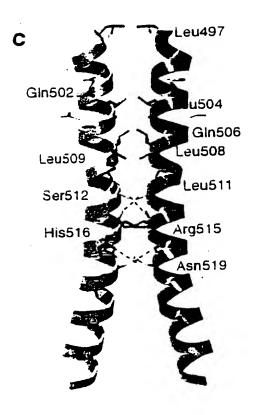


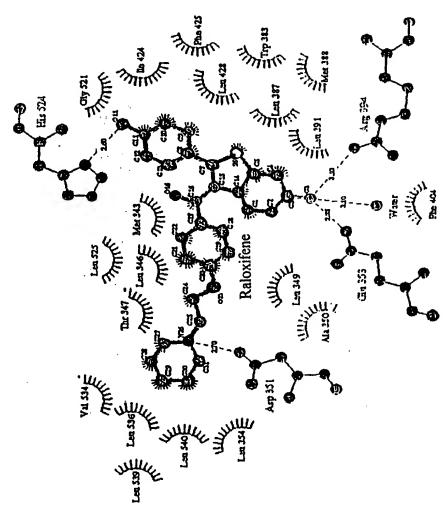


SUBSTITUTE SHEET (RULE 26)

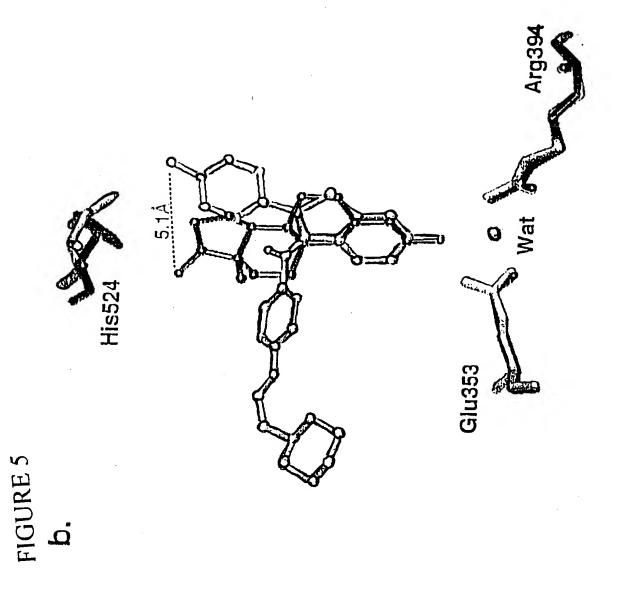


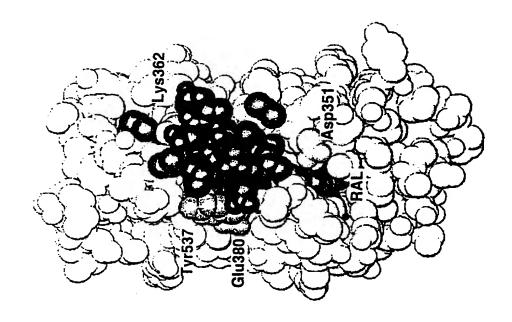
## FIGURE 4





FIC





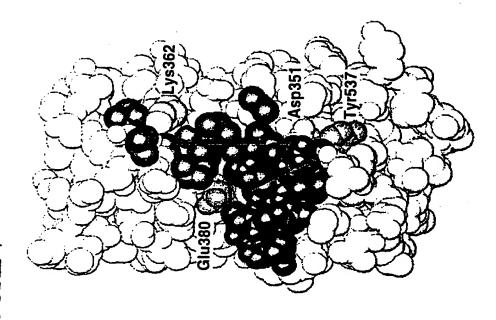


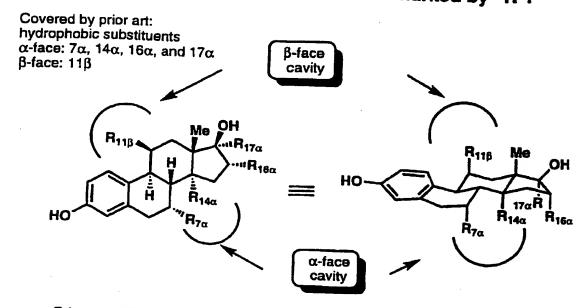
FIGURE 7

## FIGURE 8

Zearalenone

Zindoxifen

# Figure 8a: affinity enhancing substituents marked by "R".



Prior art reviewed in "The estradiol pharmacophore: ligand structure-estrogen receptor binding affinity relationships" G.M. Anstead, K.E. Carlson, and J.A. Katzenellenbogen, Steroids, 62(3):268-303 (1997).

## Figure 8b: affinity enhancing substituents marked by "R".

Not covered by prior art: hydrophobic substituents 
$$\alpha$$
-face:  $9\alpha$  and  $12\alpha$   $\beta$ -face:  $9\alpha$  and  $12\alpha$   $\beta$ -face:  $8\beta$ ,  $15\beta$ , and  $18$   $R_{12\alpha}$   $R_{18}$   $R_{19}$   $R_$ 

### Figure 8c: affinity enhancing substituents marked by "R".

Figure 8d: affinity enhancing substituents. Replacement of 4'-OH group in raloxifene with 4'-NH<sub>2</sub> provides the opportunity of picking up an additional hydrogen bond to His-524.

Figure 8e: guanidino affinity enhancing substituent at position-3 of the steroid nucleus and position-6 of the benzothiophene nucleus.

Figure 9a: selectivity enhancing substituents R<sub>3</sub>, R<sub>2</sub>', R<sub>3</sub>', and R<sub>6</sub>'.

$$\alpha$$
-face Lew/Met-384

Ho R<sub>3</sub> R<sub>2</sub>' R<sub>3</sub>' His-524

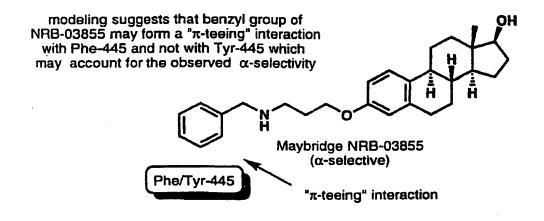
 $\beta$ -face Met/Ile-421

 $R_3$ ,  $R_2$ ',  $R_3$ ', and  $R_6$ ' = Cl, Br, I, Me, Et, *i*-Pr, and perfluoro Me, Et, and *i*-Pr.

Figure 9b: selectivity enhancing substituents  $R_3$ ,  $R_2$ ',  $R_3$ ', and  $R_6$ '. Movement of hydroxyl from position-4' to -5' biases binding orientation and therefore further enhances selectivity.

 $R_3$ ,  $R_2$ ,  $R_3$ , and  $R_6$  = Cl, Br, l, Me, Et, *i*-Pr, and perfluoro Me, Et, and *i*-Pr.

#### Figure 9c: selectivity enhancing substituents R<sub>3</sub>.



#### Figure 9d: selectivity enhancing substituents R<sub>6</sub>.

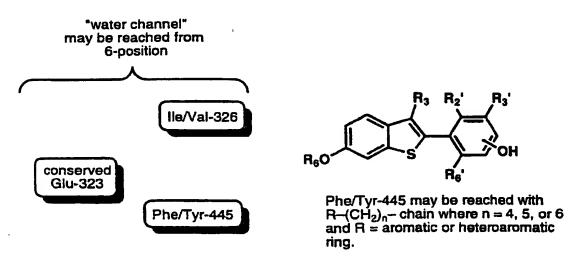
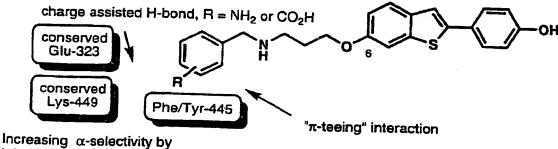


Figure 9e: selectivity enhancement reinforced by charged assisted hydrogen bond betwen substitutient "R" in the ligand and either Glu-323 or Lys-449 in the receptor.



Increasing α-selectivity by reinforcing Phe-445 interaction with H-bonding to Glu-323

Figure 9f: selectivity enhancement reinforced by hydrogen bond network between pyridone ring in the ligand and residues Glu-323 and Lys-449 in the receptor.

## FIGURE 10

25, 24, 25, 21, 21, 17, 17, 15, 11, 11, 11, 11, 10, 9, 7, 6, 6, 7, 19, 21, 23, 24, 25, 26

# FIGURE 10 continued

## FIGURE 11

#### Example 16,18

## FIGURE 12

## FIGURE 13

#### Example 22

## FIGURE 14

Example 28, 29, 30, 31, 32, 35, 37, 38, 39, 40, 45

## FIGURE 15

## FIGURE 16

## FIGURE 17

#### Example 41, 42, 43

FIGURE 18

27/371

Example 46, 47, 48

## FIGURE 19

Example 49, 50, 51

FIGURE 20 29/371

HEADER NUCLEAR RECEPTOR 08-SEP-97 1ERR COMPND MOL\_ID: 1; COMPND 2 MOLECULE: OESTROGEN RECEPTOR; COMPND 3 CHAIN: A, B; COMPND 4 FRAGMENT: LIGAND-BINDING DOMAIN; COMPND 5 SYNONYM: ESTROGEN RECEPTOR, ER-LBD; COMPND 6 ENGINEERED: YES; COMPND 7 BIOLOGICAL\_UNIT: DIMER; COMPND 8 OTHER\_DETAILS: LIGAND-BINDING DOMAIN COMPND 9 (DOMAIN E - RESIDUES 301-553) IN COMPLEX WITH THE SELECTIVE COMPND 10 ANTAGONIST RALOXIFENE SOURCE MOL\_ID: 1; SOURCE 2 ORGANISM SCIENTIFIC: HOMO SAPIENS; SOURCE 3 ORGANISM\_COMMON: HUMAN; SOURCE 4 STRAIN: JM109; SOURCE 5 VARIANT: C1857; SOURCE 6 PLASMID: PEALPHA 35; SOURCE 7 GENE: ER ALPHA; SOURCE 8 EXPRESSION SYSTEM: ESCHERICHIA COLI; SOURCE 9 EXPRESSION\_SYSTEM\_STRAIN: JM109; SOURCE 10 EXPRESSION SYSTEM\_VARIANT: C1857; SOURCE 11 EXPRESSION\_SYSTEM PLASMID: PEALPHA 35 AUTHOR A.M.BRZOZOWSKI, A.C.W.PIKE JRNL AUTH A.M.BRZOZOWSKI, A.C.W.PIKE, Z.DAUTER, R.E.HUBBARD, JRNL AUTH 2 T.BONN, O.ENGSTROM, L.OHMAN, G.L. GREENE, JRNL AUTH 3 J.-A.GUSTAFFSON,M.CARLQUIST
JRNL TITL MOLECULAR BASIS OF AGONISM AND ANTAGONISM IN THE JRNL TITL 2 OESTROGEN RECEPTOR JRNL REF TO BE PUBLISHED 0353 JRNL REFN ASTM REMARK 1 REMARK 2 REMARK 2 RESOLUTION. 2.6 ANGSTROMS. REMARK 3 REMARK 3 REFINEMENT. REMARK 3 PROGRAM : REFMAC REMARK 3 AUTHORS : MURSHUDOV, VAGIN, DODSON REMARK 3 REMARK 3 DATA USED IN REFINEMENT. REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS): 2.6 REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS): 25 REMARK 3 DATA CUTOFF (SIGMA(F)): 0 REMARK 3 COMPLETENESS FOR RANGE (%): 95.7 : 15433 REMARK 3 NUMBER OF REFLECTIONS REMARK 3

REMARK 3 FIT TO DATA USED IN REFINEMENT.

REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE (WORKING + TEST SET) : NONE
REMARK 3 R VALUE (WORKING SET) : 0.219
REMARK 3 FREE R VALUE : 0.299
REMARK 3 FREE R VALUE TEST SET SIZE (%) : 10
REMARK 3 FREE R VALUE TEST SET COUNT : 1565
REMARK 3
REMARK 3
REMARK 3
NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.

REMARK 3 PROTEIN ATOMS : 3553
REMARK 3 NUCLEIC ACID ATOMS : 0
REMARK 3 HETEROGEN ATOMS : 80
REMARK 3 SOLVENT ATOMS : 100

REMARK 3 REMARK 6

REMARK 6 ER-LBD WAS CARBOXYMETHYLATED PRIOR TO

CRYSTALLISATION. ONLY

REMARK 6 THE CARBOXYMETHYL GROUP BOUND TO CYS 381 COULD BE CLEARLY

REMARK 6 LOCATED IN THE MAPS. THIS GROUP IS PRESENTED IN THE

REMARK 6 COORDINATE FILE AS HET GROUP CBM 381 AT THE END OF EACH

REMARK 6 CHAIN.

REMARK 7

REMARK 7 RESIDUES TYR331(A), ASP332(A), HIS377(B), GLU397(AB),

REMARK 7 LYS416(AB), GLU419(AB), GLU423(B), LEU469(B), GLU470(AB), GLU471

REMARK 7 (AB),LYS472(AB),ARG477(AB),LYS492(A),LYS529(B),GLU542(A),

REMARK 7 ARG548(B) AND LEU549(B) WERE POORLY RESOLVED IN THE ELECTRON

REMARK 7 DENSITY MAPS AND ARE NOT FULLY MODELLED IN THIS ENTRY.

**REMARK 8** 

REMARK 8 RESIDUES MODELLED IN ALTERNATE CONFORMATIONS: A373,A377,

REMARK 8 A381,A473,A501,B455-B457,B501,B526.

REMARK 999

**REMARK 999 SEQUENCE** 

REMARK 999 REFERENCE: SER A 301 - LEU A 306 MISSING FROM PDB DUE TO DISORDER

REMARK 999 REFERENCE: THR A 460 - LEU A 469 MISSING FROM PDB DUE TO DISORDER

REMARK 999 REFERENCE: LYS A 529 - VAL A 534 MISSING FROM PDB DUE TO DISORDER

REMARK 999 REFERENCE: ARG A 548 - THR A 553 MISSING FROM PDB DUE TO DISORDER

REMARK 999 REFERENCE: SER B 301 - SER B 305 MISSING FROM PDB DUE TO DISORDER REMARK 999 REFERENCE: ASP B 332 - GLU B 339 MISSING FROM PDB DUE TO DISORDER REMARK 999 REFERENCE: THR B 460 - SER B 468 MISSING FROM PDB DUE TO DISORDER REMARK 999 REFERENCE: CYS B 530 - PRO B 535 MISSING FROM PDB DUE TO DISORDER REMARK 999 REFERENCE: PRO B 552 - THR B 553 MISSING FROM PDB DUE TO DISORDER SG ACYS A 381 LINK C2 ACBM A 381 SG BCYS A 381 LINK C2 ACBM A 381 SG ACYS A 381 C2 BCBM A 381 LINK SG BCYS A 381 LINK C2 BCBM A 381 SG CYS B 381 LINK C2 CBM B 381 CISPEP ! ARG A 335 PRO A 336 0 0.13 CRYST1 104.530 53.680 102.710 90.00 116.79 90.00 C 1 2 1 ORIGX1 1.000000 0.000000 0.000000 0.00000 0.000000 1.000000 0.000000 0.00000 ORIGX2 ORIGX3 0.000000 0.000000 1.000000 0.00000 SCALE1 0.009567 0.000000 0.004830 0.00000 0.000000 0.018629 0.000000 0.00000 SCALE2 SCALE3 0.000000 0.000000 0.010907 0.00000 MTRIX1 1 -0.740953 -0.502251 0.445794 74.86100 1 MTRIX2 1 -0.502316 -0.026089 -0.864290 122.90400 1 94.95000 1 MTRIX3 1 0.445721 -0.864328 -0.232958 1 N ALA A 307 54.098 63.501 73.107 1.00101.44 N ATOM C 2 CA ALA A 307 53.995 62.069 72.653 1.00101.06 ATOM 3 C ALA A 307 52.966 61.945 71.536 1.00100.17 C ATOM O ATOM 4 O ALA A 307 53.280 61.646 70.377 1.00 99.09 ATOM 5 CB ALA A 307 53.690 61.140 73.815 1.00100.89 C N 6 N LEU A 308 51.722 62,276 71.868 1.00 99.53 ATOM C 50.596 62.259 70.953 1.00 99.09 7 CA LEU A 308 ATOM C 50.516 63.528 70.121 1.00 98.93 8 C LEU A 308 ATOM 0 49.540 63.825 69.426 1.00100.59 9 O LEU A 308 ATOM C 49.302 62.048 71.772 1.00 98.27 10 CB LEU A 308 ATOM C 49.294 60.672 72.455 1.00 98.34 11 CG LEU A 308 ATOM C 48,270 60,564 73,564 1.00 99.10 ATOM 12 CD1 LEU A 308 C 49.073 59.608 71.396 1.00 99.05 ATOM 13 CD2 LEU A 308 N 51.593 64.289 70.149 1.00 97.52 ATOM 14 N SER A 309 51.799 65.546 69.479 1.00 94.74 C 15 CA SER A 309 ATOM C 52.762 65.407 68.308 1.00 90.63 ATOM 16 C SER A 309 53.020 66.365 67.590 1.00 91.89 0 ATOM 17 O SER A 309 C 52.357 66.583 70.456 1.00 96.58 18 CB SER A 309 ATOM 0 19 OG SER A 309 52.346 66.102 71.800 1.00100.04 ATOM 53.298 64.214 68.092 1.00 85.74 N 20 N LEU A 310 ATOM C 54.212 64.025 66.973 1.00 80.17 21 CA LEU A 310 ATOM 53.475 63.652 65.701 1.00 75.60 C 22 C LEU A 310 ATOM 0

23 O LEU A 310

52.519 62.877 65.644 1.00 75.27

ATOM

		•	
ATOM	24 CB LEU A 310	55,259 62,961 67,314 1,00 82,19	С
<b>ATOM</b>	25 CG LEU A 310	56.128 63.380 68.513 1.00 84.04	С
ATOM	26 CD1 LEU A 310	56,916 62,196 69,021 1,00 85,21	С
ATOM	27 CD2 LEU A 310	57.028 64.542 68.119 1.00 85.94	С
ATOM	28 N THR A 311	53.925 64.277 64.620 1.00 69.23	N
ATOM	29 CA THR A 311	53.347 64.005 63.307 1.00 65.09	С
ATOM	30 C THR A 311		C
ATOM	31 O THR A 311	54.838 62.147 63.496 1.00 56.82	0
ATOM		53.884 64.913 62.189 1.00 66.58	C
ATOM		55.198 64.441 61.861 1.00 67.83	O
ATOM		53,990 66,380 62,503 1,00 66,63	Č
ATOM	35 N ALA A 312		N
ATOM	36 CA ALA A 312		C
ATOM	37 C ALA A 312		C
ATOM	38 O ALA A 312	55.871 59.918 61.816 1.00 55.73	ŏ
ATOM	39 CB ALA A 312	53.021 60.320 60.154 1.00 55.64	Č
ATOM	40 N ASP A 313		N
ATOM		57.000 61.809 60.232 1.00 61.36	C
ATOM	42 C ASP A 313		C
ATOM	43 O ASP A 313	58.925 61.401 61.501 1.00 59.92	Ō
ATOM		57.421 62.678 59.065 1.00 66.00	C
ATOM		56.760 62.221 57.760 1.00 70.36	C
ATOM		57.126 61.157 57.216 1.00 69.20	0
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ATOM	49 CA GLN A 314		C
ATOM	50 C GLN A 314		C
ATOM	51 O GLN A 314		O
ATOM	52 CB GLN A 314	57.673 64.099 64.529 1.00 68.68	С
ATOM		57.411 65.462 63.876 1.00 72.34	С
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ATOM	62 CG MET A 315	55.573 57.619 65.179 1.00 61.37	C
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ATOM	66 CA VAL A 316	59.184 57.774 62.491 1.00 50.51	С
ATOM	67 C VAL A 316	60,656 58.049 62.696 1.00 49,96	С
ATOM	68 O VAL A 316	61.451 57.091 62.811 1.00 50.67	Ö
ATOM	69 CB VAL A 316	58.854 57.823 60.983 1.00 52.04	C
ATOM	70 CG1 VAL A 316	59.711 56.828 60.214 1.00 51.77	C
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ATOM	72 N SER A 317	61.003 59.331 62.639 1.00 48.06	N
	· <del></del>		

		•	
ATOM	73 CA SER A 317	62.423 59.721 62.777 1.00 48.67	С
ATOM	74 C SER A 317	62.813 59.525 64.238 1.00 47.57	С
ATOM	75 O SER A 317	63.778 58.816 64.595 1.00 48.05	0
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ATOM	77 OG SER A 317	61.339 61.700 63.181 1.00 54.05	O
<b>ATOM</b>	78 N ALA A 318	62.000 60.024 65.158 1.00 43.79	N
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ATOM	80 C ALA A 318	62.622 58.278 66.738 1.00 46.07	С
ATOM	81 O ALA A 318	63.724 57.937 67.164 1.00 48.86	O
ATOM	82 CB ALA A 318	60.958 60.040 67.312 1.00 43.54	С
ATOM	83 N LEU A 319	61.721 57.372 66.259 1.00 44.84	N
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ATOM	85 C LEU A 319	63.249 55,560 65.808 1.00 41.35	С
ATOM	86 O LEU A 319	64.114 54.940 66.442 1.00 43.08	О
<b>ATOM</b>		60.818 55.095 66.132 1.00 35.20	С
ATOM	88 CG LEU A 319	59.455 55.190 66.778 1.00 34.47	С
<b>ATOM</b>	89 CD1 LEU A 319		C
<b>ATOM</b>	90 CD2 LEU A 319	59.388 54.770 68.217 1.00 28.80	С
<b>ATOM</b>	91 N LEU A 320	63.462 55.915 64.567 1.00 46.80	N
<b>ATOM</b>	92 CA LEU A 320	64.721 55.511 63.886 1.00 48.28	С
<b>ATOM</b>	93 C LEU A 320	65.946 55.905 64.667 1.00 49.61	С
<b>ATOM</b>	94 O LEU A 320	66.922 55.170 64.714 1.00 50.99	0
<b>ATOM</b>		64.715 56.108 62.472 1.00 48.30	С
<b>ATOM</b>	96 CG LEU A 320	63.875 55.286 61.483 1.00 49.80	С
<b>ATOM</b>	97 CD1 LEU A 320	63.709 55.967 60.158 1.00 49.05	С
<b>ATOM</b>	98 CD2 LEU A 320	64.519 53.925 61.255 1.00 51.04	С
<b>ATOM</b>	99 N ASP A 321	65.935 57.068 65.308 1.00 53.09	N
<b>ATOM</b>	100 CA ASP A 321		С
<b>ATOM</b>	101 C ASP A 321	67.294 56.752 67.337 1.00 48.52	C
<b>ATOM</b>	102 O ASP A 321	68.447 56.506 67.654 1.00 52.66	0
<b>ATOM</b>		66.739 59.000 66.649 1.00 57.98	C
<b>ATOM</b>		67.872 59.919 66.255 1.00 63.89	C
<b>ATOM</b>	105 OD1 ASP A 321	68.362 59.817 65.107 1.00 66.13	0
<b>ATOM</b>	106 OD2 ASP A 321	68.276 60.724 67.122 1.00 69.06	0
<b>ATOM</b>	107 N ALA A 322	66.228 56.278 67.943 1.00 41.85	N
<b>ATOM</b>	108 CA ALA A 322	66.295 55.442 69.123 1.00 36.67	С
<b>ATOM</b>	109 C ALA A 322	66.794 54.049 68.847 1.00 33.38	C
<b>ATOM</b>	110 O ALA A 322	66,970 53,238 69,749 1.00 34.81	0
<b>ATOM</b>	111 CB ALA A 322	64.909 55.394 69.764 1.00 36.73	С
<b>ATOM</b>	112 N GLU A 323	67.078 53.724 67.616 1.00 31.88	N
<b>ATOM</b>	113 CA GLU A 323	67.392 52.340 67.287 1.00 34.43	C
<b>ATOM</b>	114 C GLU A 323	68.526 51.925 68.094 1.00 35.40	C
ATOM	115 O GLU A 323	69.427 52.756 68.242 1.00 44.66	0
ATOM	116 CB GLU A 323	67.529 52.209 65.773 1.00 35.17	C
ATOM	117 CG GLU A 323		C
ATOM	118 CD GLU A 323		C
ATOM	119 OE1 GLU A 323		0
ATOM	120 OE2 GLU A 323		.0
ATOM	121 N PRO A 324	68.537 50.780 68.697 1.00 37.20	N

	· •		
ATOM	122 CA PRO A 324 6	59.755 50.328 69.431 1.00 37.25	С
ATOM	123 C PRO A 324 70	0.811 50.012 68.373 1.00 37.44	С
ATOM	124 O PRO A 324 70	0.483 49.787 67.218 1.00 38.76	0
ATOM	125 CB PRO A 324 6	9.416 49.034 70.128 1.00 33.21	С
ATOM		58.160 48.636 69.459 1.00 33.49	С
ATOM	127 CD PRO A 324	57.551 49.752 68.621 1.00 34.65	С
ATOM		2.044 49.948 68.804 1.00 36.23	N
ATOM		73.174 49.603 67.970 1.00 34.39	С
ATOM		3,223 48,132 67,679 1,00 36,48	С
ATOM		2.707 47.405 68.550 1.00 43.04	0
ATOM		74.395 49.931 68.883 1.00 30.34	С
ATOM		73.826 49.651 70.222 1.00 33.20	С
ATOM		72.412 50.153 70.200 1.00 35.18	С
ATOM	135 N ILE A 326 73	.844 47.574 66.682 1.00 37.00	N
ATOM		3.891 46.094 66.592 1.00 35.96	С
ATOM		.121 45.635 67.301 1.00 39.02	С
ATOM		.214 46.058 66.903 1.00 47.09	0
ATOM		3.877 45.664 65.119 1.00 37.18	С
ATOM		2.440 45.960 64.571 1.00 33.71	С
ATOM		74.228 44.209 64.877 1.00 34.30	С
ATOM		72.322 45.838 63.110 1.00 32.65	С
ATOM		5.061 44.831 68.339 1.00 38.76	N
ATOM		76.223 44.386 69.099 1.00 33.89	C.
ATOM		5.869 43.164 68.493 1.00 37.30	С
ATOM	•	6.300 42.514 67.653 1.00 35.59	0
ATOM		75.761 44.038 70.533 1.00 31.03	С
ATOM		75.027 45.176 71.259 1.00 31.56	С
ATOM		74.951 44.900 72.762 1.00 28.63	С
ATOM		75.747 46.531 71.068 1.00 29.79	С
ATOM		8.065 42.777 68.973 1.00 39.80	N
ATOM		78.752 41.596 68.506 1.00 38.44	С
ATOM		8.791 40.517 69.572 1.00 42.46	С
ATOM		8.752 40.739 70.808 1.00 40.42	0
ATOM		80.223 41.999 68.242 1.00 39.84	С
<b>ATOM</b>	156 CG TYR A 328	80.429 42.530 66.862 1.00 44.53	C
<b>ATOM</b>	157 CD1 TYR A 328	80.133 43.840 66.561 1.00 46.24	С
ATOM		80.912 41.696 65.840 1.00 48.79	С
ATOM		80.305 44.316 65.284 1.00 50.15	С
<b>ATOM</b>	160 CE2 TYR A 328	81.078 42.159 64.556 1.00 49.24	С
ATOM		80.754 43.475 64.302 1.00 52.20	С
ATOM		80.907 44.010 63.033 1.00 59.80	0
ATOM		9.057 39.298 69.107 1.00 45.70	N
ATOM		79.214 38.169 70.008 1.00 51.02	С
ATOM	· <del>-</del>	0.586 38.188 70.668 1.00 56.51	С
ATOM		1.548 38.612 70.018 1:00 55.49	0
ATOM		79.156 36.880 69.159 1.00 50.86	С
ATOM		79.310 35.775 70.062 1.00 52.63	0
ATOM	· · ·	30.706 37.683 71.878 1.00 65.75	N
ATOM		82.025 37.611 72.521 1.00 76.01	С

ATOM	171 C GLUA 330	82.960 37.133 71.396 1.00 81.00	С
ATOM	172 O GLU A 330	82,675 36.107 70.813 1.00 79.13	0
ATOM	173 CB GLU A 330		С
ATOM		80.998 36.670 74.700 1.00 84.53	C
ATOM	175 CD GLU A 330		Č
ATOM		80.793 34.362 75.470 1.00 88.61	Ö
		81.382 35.913 76.917 1.00 89.74	ŏ
ATOM		83.985 37.902 71.102 1.00 91.50	N
ATOM		84.918 37.609 70.032 1.00100.48	C
ATOM			c
ATOM	180 C TYR A 331		
ATOM	181 O TYR A 331		O . C
ATOM		86.138 38.522 70.026 1.00 99.32	
ATOM	190 N ASP A 332		N
ATOM		85.796 34.214 68.578 1.00120.41	C
ATOM	192 C ASP A 332		C
ATOM	193 O ASP A 332		0
ATOM		86.895 34.137 67.490 1.00120.22	С
ATOM		85.358 32.668 70.380 1.00128.51	N
ATOM	199 CA PRO A 333	85.716 31.776 71.485 1.00130.41	С
<b>ATOM</b>	200 C PRO A 333	86.343 30.548 70.821 1.00131.42	С
ATOM	201 O PRO A 333	87.547 30.533 70.554 1.00133.43	O
ATOM	202 CB PRO A 333	84,415 31,426 72,212 1,00130,17	С
ATOM	203 CG PRO A 333	83,390 31,669 71,139 1,00129,68	С
ATOM	204 CD PRO A 333	83,944 32,552 70,043 1,00128.77	С
ATOM	205 N THR A 334		N
ATOM		85.948 28.337 69.884 1.00129.25	С
ATOM	207 C THR A 334		С
ATOM	208 O THR A 334		0
ATOM		86.605 27.340 70.853 1.00129.94	С
ATOM	210 OG1 THR A 334		0
ATOM		88.121 27.474 70.833 1.00131.04	С
ATOM		85.107 27.111 67.999 1.00125.90	N
ATOM		84.113 26.382 67.198 1.00123.68	С
ATOM	214 C ARG A 335	84.728 25.036 66.825 1.00119.67	C
ATOM	215 O ARG A 335	85.940 24.931 66.633 1.00119.78	Ö
ATOM	216 CB ARG A 335	83.720 27.231 66.009 1.00125.31	Č
ATOM	217 CG ARG A 335	82.285 27.149 65.540 1.00127.03	Č
ATOM	217 CO ARG A 335 218 CD ARG A 335	81.655 28.529 65.578 1.00128.25	č
	218 CD ARG A 335 219 NE ARG A 335	82.347 29.451 64.686 1.00129.98	Ň
ATOM	220 CZ ARG A 335	81.682 30.315 63.921 1.00130.52	Ċ
ATOM		80.362 30.315 63.921 1.00130.32	N
ATOM	221 NH1 ARG A 335		N
ATOM	222 NH2 ARG A 335	82.367 31.123 63.131 1.00131.96	N
ATOM	223 N PRO A 336	83.912 24.016 66.729 1.00115.59	
ATOM	224 CA PRO A 336	82.489 24.100 66.951 1.00113.40	C
ATOM	225 C PRO A 336	82.114 24.304 68.410 1.00111.16	C
ATOM	226 O PRO A 336	82.732 23.804 69.352 1.00110.30	0
ATOM	227 CB PRO A 336	81.900 22.777 66.413 1.00113.87	C
ATOM	228 CG PRO A 336	83.075 21.850 66.561 1.00113.87	C
ATOM	229 CD PRO A 336	84.336 22.658 66.384 1.00114.86	С

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<b>ATOM</b>	230 N PHE A 337	81.056 25.072 68.653 1.00108.59	N
<b>ATOM</b>	231 CA PHE A 337	80.592 25.302 70.005 1.00107.41	С
ATOM	232 C PHE A 337	79.944 24.019 70.544 1.00105.98	C
ATOM	233 O PHE A 337	79.608 23.095 69.811 1.00105.97	0
ATOM	234 CB PHE A 337	79.494 26.381 70.074 1.00108.40	С
ATOM	235 CG PHE A 337	79.786 27.668 69.384 1.00109.05	С
ATOM	236 CD1 PHE A 337	80.817 28.477 69.826 1.00110.21	С
ATOM	237 CD2 PHE A 337	79.061 28.082 68.283 1.00109.60	Ç
ATOM	238 CE1 PHE A 337		Ċ
ATOM	239 CE2 PHE A 337	79.344 29.276 67.646 1.00110.17	С
ATOM	240 CZ PHE A 337	80.379 30.077 68.098 1.00110.36	С
ATOM	241 N SER A 338	79.684 24.056 71.839 1.00104.12	N
ATOM	242 CA SER A 338	78.921 23.005 72.510 1.00101.32	С
ATOM	243 C SER A 338	77.542 23.619 72.828 1.00 99.90	. C
ATOM	244 O SER A 338	77.245 24.736 72.394 1.00 98.36	0
ATOM	245 CB SER A 338	79.628 22.537 73.768 1.00 99.85	С
ATOM	246 OG SER A 338	79.630 23.506 74.795 1.00 98.71	0
ATOM	247 N GLU A 339	76.720 22.900 73.575 1.00 98.70	N
ATOM	248 CA GLU A 339		С
ATOM	249 C GLU A 339	75.629 24.565 74.947 1.00 92.79	С
ATOM	250 O GLU A 339	75.146 25.676 74.716 1.00 91.77	0
ATOM	251 CB GLU A 339	74.542 22.333 74.539 1.00101.76	С
ATOM	252 CG GLU A 339		С
ATOM	253 CD GLU A 339		Ċ
ATOM			0
ATOM	255 OE2 GLU A 339		0
<b>ATOM</b>	256 N ALA A 340	76.455 24.326 75.964 1.00 87.20	N
ATOM	257 CA ALA A 340	76,727 25.362 76.943 1.00 84.40	С
<b>ATOM</b>	258 C ALA A 340	77.497 26.557 76.397 1.00 81.16	С
<b>ATOM</b>	259 O ALA A 340	77.234 27.697 76.785 1.00 80.26	0
<b>ATOM</b>	260 CB ALA A 340	77.457 24.787 78.161 1.00 85.04	С
<b>ATOM</b>	261 N SER A 341	78.452 26.338 75.510 1.00 77.03	N
<b>ATOM</b>	262 CA SER A 341	79.267 27.403 74.926 1.00 72.02	С
<b>ATOM</b>	263 C SER A 341	78.435 28.351 74.080 1.00 67.47	С
<b>ATOM</b>	264 O SER A 341	78.568 29.576 74.162 1.00 63.26	0
<b>ATOM</b>	265 CB SER A 341	80.428 26.784 74.137 1.00 71.53	C
<b>ATOM</b>	266 OG SER A 341	80.507 27.178 72.795 1.00 69.57	0
<b>ATOM</b>	267 N MET A 342	77.581 27.768 73.248 1.00 64.08	N
<b>ATOM</b>	268 CA MET A 342	76.671 28.553 72.431 1.00 62.01	С
<b>ATOM</b>	269 C MET A 342	75.663 29.290 73.319 1.00 58.62	C
<b>ATOM</b>	270 O MET A 342	75.325 30.455 73.098 1.00 56.39	0
<b>ATOM</b>	271 CB MET A 342	75.893 27.597 71.535 1.00 62.67	С
<b>ATOM</b>	272 CG MET A 342	74.882 28.258 70.647 1.00 63.17	С
<b>ATOM</b>	273 SD MET A 342	74.747 27.389 69.098 1.00 70.28	S
<b>ATOM</b>	274 CE MET A 342		С
<b>ATOM</b>	275 N MET A 343	75.190 28.560 74.346 1.00 52.89	N
<b>ATOM</b>	276 CA MET A 343	74.213 29.182 75.229 1.00 50.63	С
<b>ATOM</b>	277 C MET A 343	74.848 30.415 75.855 1.00 49.91	С
ATOM	278 O MET A 343	74.196 31.460 75.988 1.00 52.56	Ο

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ATOM	279 CB MET A 343		C
ATOM	280 CG MET A 343	72,421 27.408 75.889 1.00 53.30	С
<b>ATOM</b>	281 SD MET A 343	71.438 28.002 74.494 1.00 60.64	S
<b>ATOM</b>	282 CE MET A 343	70.677 29.482 75.224 1.00 52.97	C
<b>ATOM</b>	283 N GLY A 344	76.090 30.324 76.252 1.00 46.32	N
ATOM	284 CA GLY A 344	76.894 31.341 76.853 1.00 40.89	C
ATOM	285 C GLY A 344	77.069 32.501 75.904 1.00 41.62	С
ATOM	286 O GLY A 344	76.845 33.648 76.313 1.00 43.99	Ο
ATOM	287 N LEU A 345	77.379 32.229 74.635 1.00 40.05	N
ATOM	288 CA LEU A 345	77.512 33.370 73.724 1.00 39.66	С
ATOM	289 C LEU A 345	76.152 34.018 73.593 1.00 42.22	С
ATOM	290 O LEU A 345	75.967 35.236 73.827 1.00 40.01	0
ATOM	291 CB LEU A 345	78.094 32.904 72.411 1.00 40.52	С
<b>ATOM</b>	292 CG LEU A 345	79.509 32.281 72.578 1.00 36.81	С
ATOM	293 CD1 LEU A 345	79.728 31.405 71.412 1.00 35.07	С
ATOM	294 CD2 LEU A 345	80.562 33.373 72.617 1.00 35.91	С
<b>ATOM</b>	295 N LEUA 346	75.135 33.152 73.330 1.00 40.70	N
ATOM	296 CA LEU A 346	73.799 33.771 73.251 1.00 38.15	С
ATOM	297 C LEU A 346	73.411 34.515 74.514 1.00 37.81	С
<b>ATOM</b>	298 O LEU A 346	72.763 35.589 74.387 1.00 33.78	· O
<b>ATOM</b>	299 CB LEU A 346	72.812 32.717 72.775 1.00 36.63	С
<b>ATOM</b>	300 CG LEU A 346	73.197 32.163 71.396 1.00 36.54	С
<b>ATOM</b>	301 CD1 LEU A 346	72.319 30.952 71.093 1.00 39.38	С
<b>ATOM</b>	302 CD2 LEU A 346	73.117 33.221 70.327 1.00 34.92	С
ATOM	303 N THR A 347	73.767 34.006 75.697 1.00 35.86	N
<b>ATOM</b>	304 CA THR A 347	73.329 34.644 76.950 1.00 38.36	С
<b>ATOM</b>	305 C THR A 347	74.041 35.977 77.122 1.00 39.47	С
<b>ATOM</b>	306 O THR A 347	73.402 36.976 77.407 1.00 40.21	0
<b>ATOM</b>	307 CB THR A 347	73.610 33.797 78.194 1.00 38.11	C
<b>ATOM</b>	308 OG1 THR A 347	73.118 32.465 78.023 1.00 43.41	0
<b>ATOM</b>	309 CG2 THR A 347	73.043 34.344 79.455 1.00 32.94	С
<b>ATOM</b>	310 N ASN A 348	75,364 35.950 76.915 1.00 38.84	N
<b>ATOM</b>	311 CA ASN A 348	76.138 37.179 77.003 1.00 35.12	С
ATOM		75.528 38.199 76.057 1.00 31.75	C
ATOM		75.185 39.266 76.531 1.00 32.58	0
ATOM		77.627 36.954 76.674 1.00 39.35	C
ATOM		78.368 38.293 76.687 1.00 43.83	C
ATOM		78.520 38.958 75.647 1.00 47.22	0
ATOM		78.692 38.727 77.886 1.00 44.28	N
ATOM		75.332 37.861 74.793 1.00 29.26	N
ATOM		74.787 38.795 73.811 1.00 27.91	C
ATOM		73.486 39:418 74.289 1.00 31.58	C
ATOM		73.345 40.634 74.458 1.00 30.15	0
ATOM		74.719 38.088 72.472 1.00 28.75	C
ATOM		74.083 38.806 71.284 1.00 36.78	C
ATOM		74.865 40.076 70.945 1.00 36.43	C
ATOM		74.014 37.922 70.034 1.00 36.80	C
ATOM		72.447 38.621 74.572 1.00 32.99	N
ATOM	327 CA ALA A 350	71.158 39.047 75.016 1.00 32.50	С

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ATOM	328 C ALA A 350	71.244 40.028 76.184 1.00 34.81	С
ATOM	329 O ALA A 350	70.514 41.032 76.293 1.00 31.47	0
ATOM	330 CB ALA A 350	70.422 37.775 75.508 1.00 34.40	С
ATOM	331 N ASP A 351	72.157 39.696 77.119 1.00 35.11	N
ATOM	332 CA ASP A 351	72.290 40.545 78.304 1.00 36.10	С
<b>ATOM</b>	333 C ASP A 351	72.844 41.893 77.939 1.00 35.62	С
ATOM	334 O ASP A 351		Ο
<b>ATOM</b>	335 CB ASP A 351		С
ATOM	336 CG ASP A 351		С
ATOM	337 OD1 ASP A 351	71.138 38.538 79.792 1.00 45.88	0
<b>ATOM</b>	338 OD2 ASP A 351	73.077 37.876 80.611 1.00 50.85	0
<b>ATOM</b>	339 N ARG A 352	73.813 41.873 77.039 1.00 34.29	N
<b>ATOM</b>	340 CA ARG A 352	74,360 43,182 76,651 1,00 30,27	С
<b>ATOM</b>	341 C ARG A 352	73.280 43.905 75.885 1.00 32.48	С
<b>ATOM</b>	342 O ARG A 352		0
<b>ATOM</b>	343 CB ARG A 352	75.659 42.934 75.942 1.00 26.80	C
ATOM	344 CG ARG A 352		C
ATOM	345 CD ARG A 352		С
<b>ATOM</b>	346 NE ARG A 352		N
<b>ATOM</b>	347 CZ ARG A 352		С
ATOM	348 NH1 ARG A 352		N
ATOM	349 NH2 ARG A 352		N
ATOM	350 N GLU A 353	72.544 43.238 74.999 1.00 33.29	N
<b>ATOM</b>	351 CA GLU A 353		С
ATOM	352 C GLU A 353		С
ATOM	353 O GLU A 353	69.862 45.515 74.941 1.00 32.80	0
ATOM	354 CB GLU A 353		C
<b>ATOM</b>	355 CG GLU A 353		C
ATOM	356 CD GLU A 353		C
ATOM	357 OE1 GLU A 353		0
ATOM	358 OE2 GLU A 353		0
ATOM	359 N LEU A 354	70.152 43.627 76.217 1.00 30.45	N
ATOM	360 CA LEU A 354	69.120 44.156 77.132 1.00 33.42	C
ATOM	361 C LEU A 354	69.419 45.557 77.625 1.00 33.94	C.
ATOM	362 O LEU A 354	68.543 46.397 77.897 1.00 35.63	0
ATOM	363 CB LEU A 354	68.904 43.225 78.282 1.00 35.57	C
ATOM	364 CG LEU A 354		C
ATOM	365 CD1 LEU A 354		C
ATOM	366 CD2 LEU A 354		C
ATOM	367 N VAL A 355	70,709 45,904 77,740 1.00 34,11	N
ATOM	368 CA VAL A 355	71.022 47.248 78.253 1.00 29.81	C
ATOM	369 C VAL A 355	70.578 48.281 77.275 1.00 32.35	C
ATOM	370 O VAL A 355	70.082 49.363 77.548 1.00 32.21	0
ATOM	371 CB VAL A 355		C
ATOM	372 CG1 VAL A 355		C
ATOM	373 CG2 VAL A 355		C
ATOM	374 N HIS A 356	70.801 48.019 75.969 1.00 35.17	N
ATOM	375 CA HIS A 356	70.469 49.090 75.019 1.00 34.30	C
ATOM	376 C HIS A 356	68.976 49.210 74.878 1.00 37.61	С

ATOM		8.470 50.298 74.605 1.00 37.88	0
<b>ATOM</b>	378 CB HIS A 356	71.119 48.696 73.700 1.00 37.14	С
<b>ATOM</b>	379 CG HIS A 356	72.604 48.940 73.811 1.00 40.21	С
ATOM	380 ND1 HIS A 356	73.150 50.199 73.687 1.00 40.55	N
ATOM	381 CD2 HIS A 356	73.615 48.091 74.046 1.00 41.21	С
<b>ATOM</b>	382 CE1 HIS A 356	74.457 50.080 73.844 1.00 42.06	C
<b>ATOM</b>	383 NE2 HIS A 356	74.762 48.822 74.038 1.00 41.48	N
<b>ATOM</b>	384 N MET A 357	68.298 48.067 75.070 1.00 34.83	N
<b>ATOM</b>	385 CA MET A 357	66.873 48.010 74.942 1.00 34.72	С
<b>ATOM</b>	386 C MET A 357	66.214 48.979 75.895 1.00 39.56	C
ATOM	387 O MET A 357	65.178 49.613 75.547 1.00 41.07	0
<b>ATOM</b>	388 CB MET A 357	66.368 46.576 75.232 1.00 35.23	C
ATOM	389 CG MET A 357	64.941 46.399 74.752 1.00 32.18	C
ATOM	390 SD MET A 357	64.275 44.817 75.326 1.00 34.77	S
ATOM	391 CE MET A 357	65.449 43.688 74.619 1.00 34.80	С
ATOM		6.795 49.034 77.102 1.00 38.12	N
ATOM		66.256 49.963 78.081 1.00 40.67	С
ATOM		6.347 51.379 77.587 1.00 44.25	C
ATOM		55,338 52,129 77.678 1.00 48.55	0
ATOM		66.916 49.765 79.451 1.00 40.93	C
ATOM	397 CG1 ILE A 358	66.228 48.488 80.022 1.00 39.31	C
ATOM	398 CG2 ILE A 358	66.637 50.945 80.347 1.00 39.18	C
ATOM	399 CD1 ILE A 358	67.075 47.683 80.909 1.00 39.58	C
ATOM		67.514 51.758 77.039 1.00 40.76	N
ATOM		67.626 53.090 76.513 1.00 40.91	C
ATOM		66.563 53.275 75.414 1.00 39.09	C
ATOM		66.079 54.381 75.223 1.00 42.57	0
ATOM	404 CB ASN A 359	68.936 53.472 75.833 1.00 44.08	C
ATOM	405 CG ASN A 359	70.118 53.378 76.729 1.00 51.07	C
ATOM	406 OD1 ASN A 359	69.922 53.474 77.967 1.00 55.22	0
ATOM	407 ND2 ASN A 359	71.312 53.183 76.144 1.00 50.95	N N
ATOM		66.430 52.328 74.532 1.00 36.27	C
ATOM	409 CA TRP A 360	65.485 52.489 73.414 1.00 36.80	c
ATOM		64.084 52.609 73.992 1.00 40.32	Ö
ATOM		63.265 53.514 73.773 1.00 37.53	C
ATOM		65.706 51.293 72.489 1.00 32.87 64.495 51.101 71.623 1.00 36.76	Č
ATOM		64.249 51.724 70.450 1.00 35.10	C
ATOM	414 CD1 TRP A 360		Č
ATOM	415 CD2 TRP A 360	63.406 50.191 71.847 1.00 36.41	N
ATOM	416 NE1 TRP A 360	63.093 51.271 69.921 1.00 35.72 62.517 50.381 70.778 1.00 38.84	C
ATOM	417 CE2 TRP A 360	63.083 49.270 72.848 1.00 35.46	Č
ATOM	418 · CE3 TRP A 360	61.270 49.707 70.703 1.00 40.31	č
ATOM	419 CZ2 TRP A 360 420 CZ3 TRP A 360	61.888 48.580 72.776 1.00 40.51	Č
ATOM		61.007 48.822 71.707 1.00 39.13	C
ATOM		63.731 51.677 74.909 1.00 40.42	N
ATOM	422 N ALA A 361 423 CA ALA A 361	62.394 51.784 75.480 1.00 43.31	C
ATOM	423 CA ALA A 361 424 C ALA A 361	62.074 53.205 75.921 1.00 43.29	c
ATOM	424 C ALA A 361 425 O ALA A 361	60.935 53.682 75.778 1.00 40.16	Ö
ATOM	423 U ALA A 301	00.733 33.002 13.110 1.00 70.10	0

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<b>ATOM</b>	426 CB ALA A 361	62.223 50.861 76.695 1.00 44:40	С
ATOM	427 N LYS A 362	63.057 53.829 76.574 1.00 44.67	N
ATOM	428 CA LYS A 362	62.873 55.140 77.180 1.00 44.02	С
ATOM	429 C LYS A 362	62.644 56.183 76.120 1.00 44.20	С
ATOM	430 O LYS A 362	62.172 57.257 76.432 1.00 46.12	Ο
ATOM	431 CB LYS A 362	64.028 55.467 78.102 1.00 45.07	С
ATOM	432 CG LYS A 362	64,099 54,601 79,360 1,00 45,39	С
ATOM	433 CD LYS A 362	63.760 55.450 80.584 1.00 50.39	С
	434 CE LYS A 362	63.073 54.690 81.677 1.00 54.46	С
ATOM	435 NZ LYS A 362	62,697 55,356 82,942 1.00 53,54	N
ATOM	436 N ARG A 363	62.896 55.918 74.859 1.00 46.04	N
ATOM	437 CA ARG A 363	62,666 56,783 73,735 1.00 48,68	С
ATOM	438 C ARG A 363	61.350 56.466 72.999 1.00 49.08	С
ATOM	439 O ARG A 363	60.941 57.054 71.977 1.00 48.73	Ο
ATOM	440 CB ARG A 363	63.836 56.643 72.757 1.00 53.32	С
ATOM	441 CG ARG A 363	64,902 57,723 72,904 1.00 60,34	С
ATOM	442 CD ARG A 363	65.590 57.624 74.196 1.00 67.72	С
ATOM	443 NE ARG A 363		. N
ATOM	444 CZ ARG A 363	67.729 57.640 75.369 1.00 80.50	С
ATOM	445 NH1 ARG A 363		N
ATOM	446 NH2 ARG A 363	69.002 58.051 75.459 1.00 84.83	N
ATOM	447 N VAL A 364	60.623 55.453 73.448 1.00 45.49	N
ATOM	448 CA VAL A 364	59,402 55.065 72.769 1.00 47.12	С
ATOM	449 C VAL A 364	58.270 55.938 73.227 1.00 52.70	C
ATOM	450 O VAL A 364		O
ATOM	451 CB VAL A 364	59.234 53.557 72.909 1.00 43.20	C
ATOM	452 CG1 VAL A 364	58.013 52.972 72.279 1.00 40.68	C
ATOM	453 CG2 VAL A 364	60.476 52.960 72.224 1.00 44.16	C
ATOM	454 N PRO A 365	57.746 56.755 72.334 1.00 56.52	N
ATOM	455 CA PRO A 365	56.660 57.676 72.630 1.00 55.71	C
ATOM	456 C PRO A 365	55,631 57.068 73.527 1.00 57.16	C
ATOM	457 O PRO A 365	55.000 56.063 73.202 1.00 59.56	O
ATOM		56.078 58.059 71.257 1.00 56.19	С
ATOM		57.446 58.203 70.542 1.00 58.84	С
ATOM	460 CD PRO A 365	58.160 56.882 70.922 1.00 58.70	C
ATOM	461 N GLY A 366	55.450 57.650 74.711 1.00 58.05	N
ATOM	462 CA GLY A 366	54.426 57.130 75.628 1.00 56.39	С
ATOM	463 C GLY A 366	55.063 56.367 76.771 1.00 56.65	С
ATOM	464 O GLY A 366	54.553 56.398 77.893 1.00 56.35	0
ATOM	465 N PHE A 367	56.197 55.701 76.480 1.00 54.46	N
ATOM	466 CA PHE A 367	56.848 54.870 77.461 1.00 49.74	С
ATOM	467 C PHE A 367	57.198 55.574 78.738 1.00 49.68	C
ATOM	468 O PHE A 367	56.884 55.121 79.814 1.00 51.83	O
ATOM	469 CB PHE A 367	58.152 54.252 76.951 1.00 46.86	C
ATOM	470 CG PHE A 367	58.531 53.053 77.781 1.00 43.25	Č
ATOM	471 CD1 PHE A 367		Č
ATOM	472 CD2 PHE A 367		Č
ATOM	473 CE1 PHE A 367		č
ATOM	474 CE2 PHE A 367		Č
A I OW	7/4 CE2 FIE A 30/	37.702 31.977 79.300 1.00 41.37	•

ATOM	475	CZ PHE A 367	59.241 50.822 79.270 1.00 41.29	С
ATOM	476	N VAL A 368	57.867 56.700 78.636 1.00 52.26	N
ATOM	477	CA VAL A 368	58.277 57.398 79.845 1.00 55.10	С
ATOM	478	C VAL A 368	57.222 58.255 80.487 1.00 57.40	С
ATOM	479	O VAL A 368	57.476 58.969 81.463 1.00 60.79	О
ATOM	480	CB VAL A 368	59.634 58.077 79.667 1.00 55.67	С
ATOM	481	CG1 VAL A 368	59.548 59.445 79.052 1.00 54.03	С
ATOM		<b>CG2 VAL A 368</b>	60.346 58.041 81.021 1.00 57.90	C
ATOM		N ASP A 369	55.977 58.178 80.074 1.00 59.67	N
ATOM		CA ASP A 369	54.828 58.794 80.705 1.00 60.47	С
ATOM		C ASP A 369	54.346 57.792 81.755 1.00 59.94	С
ATOM	486		53.766 58.144 82.766 1.00 65.43	0
ATOM		CB ASP A 369	53.690 59.040 79.724 1.00 64.16	С
ATOM		CG ASP A 369	54.038 60.056 78.677 1.00 67.29	С
ATOM		OD1 ASP A 369		Ο
ATOM		OD2 ASP A 369		Ο
ATOM		N LEUA 370	54.608 56.510 81.531 1.00 57.33	N
ATOM		CA LEU A 370	54.194 55.517 82.497 1.00 56.12	С
ATOM		C LEU A 370	55.117 55.633 83.719 1.00 57.05	С
ATOM	494			Ο
ATOM		CB LEU A 370		С
ATOM		CG LEU A 370		С
ATOM		CD1 LEU A 370	54.145 52.344 80.254 1.00 49.81	С
ATOM		CD2 LEU A 370	52.260 53.992 80.522 1.00 51.85	С
ATOM		N THR A 371	54.648 55.068 84.805 1.00 57.19	N
ATOM		CA THR A 371	55.305 54.930 86.062 1.00 54.21	С
ATOM	501	C THR A 371	56.361 53.825 85.887 1.00 56.67	С
ATOM	502	O THR A 371	56,131 52.858 85.158 1.00 55.41	0
ATOM		CB THR A 371		С
ATOM		OG1 THR A 371		0
ATOM		CG2 THR A 371		С
ATOM			57.455 53.969 86.615 1.00 57.36	N
ATOM	507	CA LEILA 372	58.566 53.062 86.620 1.00 58.29	С
ATOM	508	C LEU A 372	58.120 51.623 86.694 1.00 60.17	С
ATOM		O LEU A 372	58.503 50.771 85.878 1.00 63.49	0
ATOM		CB LEU A 372	59.497 53.427 87.759 1.00 57.98	С
ATOM		CG LEU A 372	60.669 52.498 88.043 1.00 59.29	С
ATOM		CD1 LEU A 372	61.657 52.449 86.860 1.00 56.28	С
		CD2 LEU A 372	61.371 52.966 89.312 1.00 58.46	С
ATOM		N HIS A 373	57.266 51.300 87.638 1.00 63.16	N
ATOM		CA HIS A 373	56.736 49.927 87.758 1.00 65.55	С
ATOM ATOM		C HIS A 373	55.954 49.441 86.539 1.00 57.99	С
		O HIS A 373	56.039 48.257 86.199 1.00 54.67	0
ATOM		CB HIS A 373	55.946 49.829 89.074 1.00 69.47	С
ATOM		CG AHIS A 373		С
ATOM		CG BHIS A 373	56.788 50.250 90.240 0.50 73.05	C
ATOM		ND1AHIS A 373		N
ATOM		ND1BHIS A 373	57.746 49.436 90.821 0.50 73.59	N
ATOM		CD2AHIS A 373	54.497 47.674 89.164 0.50 74.74	C
ATOM	دےد	ODEUTIO U 2/2	Ja. 17 1 11.07 1 02.10 1 0.00 1 3.1 1	

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ATOM	524 CD2BHIS A 37		С
ATOM	525 CE1AHIS A 373		С
ATOM	526 CE1BHIS A 373	58.323 50.101 91.800 0.50 74.02	С
ATOM	527 NE2AHIS A 37		N
ATOM	528 NE2BHIS A 373		N
ATOM	529 N ASP A 374		N
ATOM		54.551 49.869 84.597 1.00 51.38	С
ATOM	531 C ASP A 374	55.515 49.657 83.442 1.00 48.48	С
ATOM	532 O ASP A 374	55.319 48.767 82.638 1.00 44.30	0
ATOM	533 CB ASP A 374	53.450 50.853 84.249 1.00 50.24	С
ATOM	534 CG ASP A 374	52.230 50.420 85.062 1.00 52.68	С
ATOM	535 OD1 ASP A 374	52.218 49.208 85.463 1.00 51.70	0
ATOM	536 OD2 ASP A 374	51.373 51.283 85.253 1.00 53.06	0
<b>ATOM</b>	537 N GLN A 375	56,573 50,488 83,455 1,00 45,36	N
ATOM	538 CA GLN A 375	57.656 50.360 82.495 1.00 41.61	С
<b>ATOM</b>	539 C GLN A 375	58.283 48.993 82.695 1.00 39.41	С
<b>ATOM</b>	540 O GLN A 375		О
ATOM	541 CB GLN A 375		С
ATOM	542 CG GLN A 375		С
ATOM	543 CD GLN A 375		С
ATOM	544 OE1 GLN A 37:		0
ATOM	545 NE2 GLN A 37		N
ATOM	546 N VAL A 376		N.
ATOM	547 CA VAL A 376		C
ATOM	548 C VAL A 376		C
ATOM	549 O VAL A 376		0
ATOM	550 CB VAL A 376		C
ATOM	551 CG1 VAL A 376		C C
ATOM	552 CG2 VAL A 376		_
ATOM	553 N HIS A 377	56.969 46.410 83.927 1.00 44.51	N C
ATOM		56.027 45.407 83.467 1.00 46.78	C
ATOM	555 C HIS A 377 556 O HIS A 377	56.050 45.247 81.960 1.00 42.12 56.204 44.128 81.478 1.00 40.13	0
ATOM	557 CB HIS A 377		C.
ATOM ATOM	558 CG AHIS A 377		C
ATOM	559 CG BHIS A 377		Č
ATOM	560 ND1AHIS A 37		N
ATOM	561 ND1BHIS A 37		N
ATOM	562 CD2AHIS A 37		C
ATOM	563 CD2BHIS A 37		C
ATOM	564 CE1AHIS A 37		Ċ
ATOM	565 CE1BHIS A 37		С
ATOM	566 NE2AHIS A 37		N
ATOM	567 NE2BHIS A 37		N
ATOM	568 N LEUA 378		N
ATOM	569 CA LEU A 378		С
ATOM	570 C LEUA 378		С
ATOM	571 O LEUA 378		Ο
ATOM	572 CB LEU A 378	55.891 47.583 79.166 1.00 35.55	С

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ATOM		54.472 48.193 79.308 1.00 35.81	C
ATOM		54.392 49.470 78.484 1.00 30.30	C
ATOM		53.362 47.280 78.812 1.00 31.78	C
ATOM	576 N LEU A 379	58.553 45.941 79.947 1.00 37.44	N
ATOM		59.758 45.222 79.522 1.00 38.20	С
ATOM	578 C LEU A 379		C
<b>ATOM</b>	579 O LEU A 379		0
ATOM		61.058 45.907 79.913 1.00 39.04	C
<b>ATOM</b>		61.325 47.100 79.006 1.00 39.22	C
<b>ATOM</b>		62.112 48.158 79.710 1.00 42.38	C
<b>ATOM</b>	583 CD2 LEU A 379	62.004 46.589 77.765 1.00 41.99	С
<b>ATOM</b>	584 N GLU A 380	59.450 43.551 81.214 1.00 40.36	N
<b>ATOM</b>	585 CA GLU A 380		С
<b>ATOM</b>	586 C GLU A 380		C
<b>ATOM</b>	587 O GLU A 380		.0
ATOM	588 CB GLU A 380	58.749 42.072 83.019 1.00 44.70	C
ATOM	589 CG GLU A 380		C
ATOM	590 CD GLU A 380		C
ATOM		57.640 41.190 85.359 1.00 64.57	0
ATOM	592 OE2 GLU A 380		0
ATOM	593 N CYS A 381	57.620 41.585 80.171 1.00 40.13	N
<b>ATOM</b>	594 CA CYS A 381		С
ATOM			C
ATOM	596 O CYS A 381		0
ATOM	597 CB CYS A 381		C
ATOM	598 SG ACYS A 381		S
ATOM		54.457 40.510 80.604 0.50 56.75	`S
ATOM	600 N ALA A 382		N
ATOM	601 CA ALA A 382		С
ATOM	602 C ALA A 382	59.715 41.782 75.473 1.00 40.25	С
ATOM	603 O ALA A 382		. 0
ATOM		58.042 43.529 75.430 1.00 39.43	C
ATOM	605 N TRP A 383	60.614 41.752 76.463 1.00 39.37	N
ATOM	606 CA TRP A 383	62.029 41.668 76.112 1.00 34.09	С
ATOM	607 C TRP A 383	62.359 40.622 75.103 1.00 31.78	С
ATOM		63.015 40.905 74.096 1.00 32.20	0
ATOM		62.859 41.672 77.383 1.00 35.92	C C
ATOM	610 CG TRP A 383	62.819 40.332 78.083 1.00 36.18	C
ATOM	611 CD1 TRP A 383	61.988 39.877 79.045 1.00 33.74	C
ATOM		63.738 39.252 77.793 1.00 32.73	N
ATOM		62.314 38.588 79.374 1.00 31.23	
ATOM		63.379 38.189 78.617 1.00 31.78	C C
ATOM		64.791 39.129 76.910 1.00 33.23	C
ATOM		64.065 36.985 78.590 1.00 34.54	C
ATOM		65.487 37.948 76.872 1.00 37.35	C
ATOM	618 CH2 TRP A 383	65.114 36.888 77.709 1.00 39.46	N
ATOM		61.904 39.399 75.220 1.00 32.57	C
ATOM		62.253 38.338 74.291 1.00 31.20	c
ATOM	621 C LEU A 384	61.644 38.543 72.923 1.00 33.24	C

ATOM	622 O LEU A 384	62.338 38.321 71.921 1.00 36.36	Ο
ATOM	623 CB LEU A 384	61.901 36.984 74.846 1.00 30.65	С
<b>ATOM</b>	624 CG LEU A 384	62.520 35.799 74.124 1.00 34.98	С
<b>ATOM</b>	625 CD1 LEU A 384	64.011 35.983 73.843 1.00 36.19	С
ATOM	626 CD2 LEU A 384	62.277 34.525 74.920 1.00 33.80	С
ATOM	627 N GLU A 385	60.426 39.016 72.851 1.00 31.93	N
<b>ATOM</b>	628 CA GLU A 385	59.761 39.353 71.602 1.00 33.94	С
ATOM	629 C GLU A 385	60.602 40.397 70.858 1.00 32.22	С
ATOM	630 O GLU A 385	60.817 40.376 69.660 1.00 33.72	Ο
ATOM	631 CB GLU A 385	58.370 39.960 71.823 1.00 35.67	С
<b>ATOM</b>	632 CG GLU A 385	57.399 39.108 72.631 1.00 38.33	С
ATOM	633 CD GLU A 385	55.994 39.641 72.528 1.00 40.58	С
ATOM	634 OE1 GLU A 385	55.547 39.798 71.400 1.00 40.46	O
ATOM	635 OE2 GLU A 385	55.290 39.935 73.508 1.00 46.27	O
<b>ATOM</b>	636 N ILE A 386	61.074 41.363 71.631 1.00 33.24	N
<b>ATOM</b>	637 CA ILE A 386	61.890 42.428 71.095 1.00 34.08	С
ATOM	638 C ILE A 386	63.252 41.946 70.640 1.00 32.42	С
ATOM	639 O ILE A 386	63.662 42.262 69.535 1.00 30.26	О
ATOM		61.988 43.548 72.115 1.00 36.86	С
ATOM	641 CG1 ILE A 386	60.540 44.052 72.312 1.00 34.58	C
ATOM	642 CG2 ILE A 386		C
ATOM	643 CD1 ILE A 386	60.405 45.082 73.399 1.00 35.95	C
ATOM	644 N LEU A 387	63.928 41.081 71.387 1.00 28.96	N.
ATOM	645 CA LEU A 387	65.174 40.562 70.881 1.00 29.61	C
ATOM	646 C LEU A 387	64.858 39.779 69.603 1.00 32.09	C
ATOM	647 O LEU A 387	65.705 39.742 68.698 1.00 34.46	0
ATOM	648 CB LEU A 387	65.889 39.569 71.835 1.00 27.75	C
ATOM	649 CG LEU A 387	66.424 40.175 73.143 1.00 26.77	C
ATOM	650 CD1 LEU A 387	67.288 39.131 73.866 1.00 23.67 67.178 41.469 72.900 1.00 20.60	C
ATOM	651 CD2 LEU A 387 652 N MET A 388	63,715 39,109 69,599 1.00 31.37	N
ATOM	653 CA MET A 388	63,407 38,271 68,455 1.00 32.11	C
ATOM ATOM	654 C MET A 388	63.407 38.271 68.433 1.00 32.11	c
ATOM	655 O MET A 388	63.618 38.897 66.152 1.00 39.16	Ö
ATOM		62.369 37.292 68.899 1.00 35.14	C
ATOM		62.997 36.132 69.696 1.00 34.54	C
ATOM	= '	61.579 35.037 70.144 1.00 31.08	S
ATOM		62.630 33.726 70.818 1.00 28.15	С
ATOM		62.163 40.064 67.378 1.00 31.76	N
ATOM	661 CA ILE A 389	61.937 40.845 66.157 1.00 28.08	С
ATOM	662 C ILE A 389	63.220 41.450 65.674 1.00 27.99	С
<b>ATOM</b>	663 O ILE A 389	63.340 41.443 64.445 1.00 33.28	0
<b>ATOM</b>	664 CB ILE A 389	60.741 41.789 66.277 1.00 29.02	С
<b>ATOM</b>	665 CG1 ILE A 389	60.019 41.955 64.912 1.00 24.45	C
<b>ATOM</b>	666 CG2 ILE A 389	61.094 43.043 67.005 1.00 24.35	С
<b>ATOM</b>	667 CD1 ILE A 389	59.099 43.122 64.867 1.00 25.54	С
<b>ATOM</b>	668 N GLY A 390	64.202 41.873 66.409 1.00 31.34	N
ATOM	669 CA GLY A 390	65.489 42.435 65.959 1.00 32.81	С
ATOM	670 C GLY A 390	66.289 41.365 65.202 1.00 37.06	С

ATOM	671 O GLY A 390	66.893 41.578 64.121 1.00 34.61	0
ATOM		56.214 40.147 65.760 1.00 36.24	N
ATOM	673 CA LEU A 391	66.917 39.020 65.149 1.00 37.58	С
ATOM		66,366 38,746 63,762 1.00 38,13	С
ATOM		66,998 38.644 62.734 1.00 41.32	0
ATOM		66.696 37.733 65.989 1.00 34.64	С
ATOM		67.358 36.473 65.437 1.00 34.89	С
ATOM		68.884 36.663 65.425 1.00 32.05	С
ATOM		67.013 35.204 66.176 1.00 30.69	С
ATOM		65.052 38.598 63.715 1.00 37.28	N
ATOM		64.396 38.272 62.452 1.00 35.17	С
ATOM	682 C VAL A 392	64.699 39.339 61.446 1.00 36.85	С
ATOM		65.135 39.107 60.309 1.00 35.69	0
ATOM		62.905 38.051 62.725 1.00 31.86	С
ATOM		62.145 38.115 61.450 1.00 33.20	С
ATOM	686 CG2 VAL A 392	62.744 36.672 63.376 1.00 29.17	С
ATOM	687 N TRP A 393	54.502 40.589 61.879 1.00 38.90	N
ATOM		64.798 41.685 60.919 1.00 40.63	C
ATOM		66.238 41.713 60.430 1.00 41.64	С
ATOM		66,577 41.830 59.234 1.00 42.66	0
ATOM		64.334 42.968 61.524 1.00 36.63	С
ATOM		64.978 44.145 60.878 1.00 41.40	С
ATOM	693 CD1 TRP A 393	66.133 44.745 61.230 1.00 42.92	С
ATOM		64.442 44.911 59.802 1.00 44.52	С
ATOM		66.348 45.849 60.435 1.00 43.05	N
<b>ATOM</b>	696 CE2 TRP A 393	65.340 45.971 59.552 1.00 44.85	С
ATOM		63.273 44.834 59.038 1.00 46.64	С
ATOM	698 CZ2 TRP A 393	65.125 46.909 58.530 1.00 47.52	C
ATOM	699 CZ3 TRP A 393		C
ATOM		63.976 46.788 57.787 1.00 46.56	С
ATOM	701 N ARG A 394	67.241 41.531 61.306 1.00 41.14	N
ATOM		68.609 41.594 60.787 1.00 38.26	С
ATOM		69.005 40.350 60.060 1.00 40.13	C
ATOM	704 O ARG A 394	70.050 40.371 59.402 1.00 44.10	0
ATOM	_	69.669 42.039 61.742 1.00 36.59	C
ATOM		70.204 41.076 62.746 1.00 34.20	С
ATOM		70.465 41.819 64.103 1.00 28.97	C
ATOM		70.926 40.678 65.024 1.00 28.34	N
ATOM		70.320 40.727 66.245 1.00 27.62	C
ATOM		69.464 41.713 66.453 1.00 19.82	N
ATOM		70.587 39.885 67.213 1.00 25.67	N
ATOM		68.208 39.318 60.111 1.00 41.76	N
ATOM	· - ·	68.452 38.051 59.429 1.00 38.35	C
ATOM		67.806 38.064 58.044 1.00 42.96	С
ATOM		68.042 37.142 57.249 1.00 43.79	0
ATOM		67.787 36.988 60.304 1.00 33.00	C
ATOM		68.581 36.712 61.393 1.00 32.59	O
ATOM		66.920 39.018 57.733 1.00 46.08	N
ATOM	719 CA MET A 396	66.241 39.028 56.474 1.00 52.16	С

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ATOM		67.080 38.719 55.245 1.00 55.78	С
ATOM		66.630 38.021 54.347 1.00 58.39	0
ATOM	722 CB MET A 396		C
ATOM	723 CG MET A 396		C
ATOM	724 SD MET A 396		S
ATOM	725 CE MET A 396		С
ATOM	726 N GLU A 397		N
ATOM	727 CA GLU A 397		С
<b>ATOM</b>	728 C GLU A 397		С
<b>ATOM</b>	729 O GLU A 397		О
<b>ATOM</b>	730 CB GLU A 397	69.836 40.417 53.676 1.00 63.51	С
<b>ATOM</b>	731 CG GLU A 397	68.932 41.412 52.969 1.00 63.47	С
<b>ATOM</b>	735 N HIS A 398	69.810 36.962 54.918 1.00 62.92	N
ATOM	736 CA HIS A 398	70.655 35.813 55.141 1.00 61.99	С
ATOM	737 C HIS A 398	69.769 34.568 55.190 1.00 63.69	С
ATOM	738 O HIS A 398		0
<b>ATOM</b>	739 CB HIS A 398	71.494 35.908 56.435 1.00 60.76	С
<b>ATOM</b>	740 CG HIS A 398	72.350 37.130 56.441 1.00 62.00	С
<b>ATOM</b>	741 ND1 HIS A 398		N
ATOM	742 CD2 HIS A 398		С
ATOM	743 CE1 HIS A 398		С
<b>ATOM</b>	744 NE2 HIS A 398	73.287 39.130 56.626 1.00 63.82	N
<b>ATOM</b>	745 N PRO A 399	69.118 34.298 54.072 1.00 64.36	N
<b>ATOM</b>	746 CA PRO A 399	68.245 33.161 53.880 1.00 63.44	С
<b>ATOM</b>	747 C PRO A 399	68.777 31.873 54.445 1.00 62.06	С
<b>ATOM</b>	748 O PRO A 399	69.878 31.459 54.055 1.00 66.41	О
<b>ATOM</b>	749 CB PRO A 399		С
<b>ATOM</b>	750 CG PRO A 399		С
ATOM	751 CD PRO A 399		С
<b>ATOM</b>	752 N GLY A 400	68.081 31.209 55.340 1.00 59.48	N
ATOM	753 CA GLY A 400		С
ATOM	754 C GLY A 400		С
ATOM	755 O GLY A 400	69.649 29.125 57.892 1.00 57.75	0
ATOM	756 N LYS A 401	69.779 31.333 57.419 1.00 60.49	N
ATOM	757 CA LYS A 401	70.647 31.575 58.580 1.00 61.65	С
ATOM	758 C LYS A 401	70.064 32.683 59.437 1.00 59.45	С
ATOM	759 O LYS A 401		0
ATOM	760 CB LYS A 401		C
ATOM	761 CG LYS A 401		C
ATOM	762 CD LYS A 401		C
ATOM	763 CE LYS A 401		С
ATOM	764 NZ LYS A 401		N
ATOM	765 N LEU A 402	70.423 32.708 60.711 1.00 52.61	N
ATOM	766 CA LEU A 402		C
ATOM	767 C LEU A 402		C
ATOM	768 O LEU A 402		0
ATOM	769 CB LEU A 402		C
ATOM	770 CG LEU A 402		C
ATOM	771 CD1 LEU A 402	2 67.769 31.650 63.986 1.00 39.53	C

66,993 33.374 62.319 1.00 39.35 C 772 CD2 LEU A 402 ATOM N 71.300 35.810 61.904 1.00 42.24 773 N LEU A 403 **ATOM** C 72.268 36.780 62.299 1.00 40.59 774 CA LEU A 403 ATOM 72.049 37.247 63.735 1.00 41.66 C 775 C LEU A 403 **ATOM** 0 71.713 38.394 64.144 1.00 41.67 776 O LEU A 403 ATOM 72.238 37.958 61.311 1.00 42.13 C 777 CB LEU A 403 ATOM C 73.447 38.895 61.429 1.00 46.14 778 CG LEU A 403 ATOM C 74.639 38.172 60.823 1.00 49.15 779 CD1 LEU A 403 ATOM C 73.227 40.203 60.714 1.00 49.49 780 CD2 LEU A 403 ATOM 72.408 36.321 64.654 1.00 40.36 N 781 N PHE A 404 ATOM 72.406 36.715 66.070 1.00 41.94 C 782 CA PHE A 404 **ATOM** C 73.318 37.929 66.247 1.00 41.94 783 C PHE A 404 **ATOM** 72.974 38.820 66.991 1.00 42.90 0 784 O PHE A 404 **ATOM** 72.843 35.598 66.931 1.00 42.78 C 785 CB PHE A 404 **ATOM** C 71.768 34.592 67.146 1.00 43.78 786 CG PHE A 404 **ATOM** C 70.810 34.769 68.112 1.00 44.40 787 CD1 PHE A 404 **ATOM** C 71.748 33.445 66.381 1.00 46.28 788 CD2 PHE A 404 ATOM C 69.841 33.791 68.313 1.00 43.91 789 CE1 PHE A 404 ATOM 70.771 32.465 66.574 1.00 44.73 C 790 CE2 PHE A 404 ATOM 69.833 32.653 67.543 1.00 43.94 C 791 CZ PHE A 404 **ATOM** N 74,436 37,946 65,571 1.00 42,52 792 N ALA A 405 **ATOM** 75.370 39.061 65.568 1.00 42.15 C 793 CA ALA A 405 ATOM 76.167 38.912 64.249 1.00 43.61 C 794 C ALA A 405 ATOM 76.106 37.832 63.651 1.00 45.81 0 795 O ALA A 405 ATOM 76,301 39.170 66.715 1.00 39.38 C 796 CB ALA A 405 **ATOM** 76.861 39.956 63.875 1.00 40.72 N 797 N PRO A 406 **ATOM** C 77.624 39.995 62.645 1.00 40.43 798 CA PRO A 406 **ATOM** C 78,662 38,899 62,665 1.00 44.15 799 C PRO A 406 **ATOM** 78.908 38.153 61.706 1.00 46.52 0 800 O PRO A 406 **ATOM** 78.192 41.408 62.548 1.00 39.43 C 801 CB PRO A 406 ATOM 77,309 42,186 63,509 1.00 38,57 C 802 CG PRO A 406 **ATOM** C 76.899 41.234 64.592 1.00 38.37 803 CD PRO A 406 ATOM 79.299 38.719 63.824 1.00 45.92 N 804 N ASN A 407 ATOM 80.292 37.685 63.991 1.00 47.14 C 805 CA ASN A 407 **ATOM** C 79.688 36.384 64.518 1.00 47.74 806 C ASN A 407 **ATOM** 80.540 35.607 64.997 1.00 49.51 0 807 O ASN A 407 **ATOM** 81.401 38.056 64.970 1.00 49.67 C 808 CB ASN A 407 ATOM C 80.967 38.449 66.364 1.00 48.87 809 CG ASN A 407 ATOM 79.848 38.858 66.629 1.00 47.25 0 810 OD1 ASN A 407 ATOM N 81,904 38,361 67,311 1,00 46,89 811 ND2 ASN A 407 ATOM 78.395 36.163 64.444 1.00 43.98 N 812 N LEU A 408 **ATOM** 77.840 34.907 64.942 1.00 44.28 C 813 CA LEU A 408 ATOM C 76.574 34.578 64.137 1.00 48.56 814 C LEU A 408 ATOM 75.483 34.720 64.657 1.00 50.61 0 815 O LEU A 408 ATOM 77.399 35.004 66.412 1.00 41.78 C 816 CB LEU A 408 ATOM C 76.965 33.709 67.060 1.00 37.59 817 CG LEU A 408 ATOM 77.962 32.592 66.735 1.00 42.03 C 818 CD1 LEU A 408 ATOM C 76.774 33.777 68.536 1.00 37.24 819 CD2 LEU A 408 ATOM 76.739 34.248 62.895 1.00 50.15 N 820 N LEU A 409 ATOM

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ATOM	821 CA LEU A 409	75.691 33.915 61.969 1.00 53.65	С
<b>ATOM</b>	822 C LEU A 409	75.440 32.418 61.915 1.00 55.29	С
<b>ATOM</b>	823 O LEU A 409	76.158 31.729 61.190 1.00 59.32	O
ATOM	824 CB LEU A 409	76.154 34.481 60.614 1.00 52.50	С
<b>ATOM</b>	825 CG LEU A 409	75.026 34.637 59.601 1.00 54.30	С
ATOM	826 CD1 LEU A 409	75.459 35.371 58.345 1.00 54.05	С
ATOM	827 CD2 LEU A 409	74.550 33.227 59.271 1.00 53.81	С
ATOM	828 N LEU A 410	74.481 31.871 62.624 1.00 55.42	N
ATOM	829 CA LEUA 410	74 215 30.453 62.637 1.00 58.30	С
ATOM	830 C LEU A 410	73.123 29.988 61.713 1.00 61.42	С
ATOM	831 O LEU A 410	72.240 30.726 61.277 1.00 62.98	О
ATOM		73.896 30.029 64.080 1.00 60.54	С
ATOM		74.877 30.535 65.147 1.00 61.88	С
ATOM	834 CD1 LEU A 410	74.560 30.031 66.548 1.00 60.79	С
ATOM		76.283 30.133 64.745 1.00 62.85	С
ATOM		73.124 28.703 61.379 1.00 64.97	N
ATOM		72.121 28.133 60.480 1.00 68.11	С
ATOM	838 C ASP A 411	71.349 27.042 61.208 1.00 70.80	С
ATOM	839 O ASP A 411	71.717 26.692 62.323 1.00 68.64	0
ATOM	' I I I I I I I I I I I I I I I I I I I	72.772 27.554 59.224 1.00 66.57	C
ATOM	841 CG ASP A 411	73.750 26.453 59.578 1.00 67.45	С
ATOM	842 OD1 ASP A 411	73.421 25.590 60.428 1.00 67.96	0
	843 OD2 ASP A 411	74.874 26.446 59.021 1.00 67.41	0
ATOM	844 N ARG A 412	70.306 26.527 60.583 1.00 78.02	N
ATOM	845 CA ARG A 412	69.449 25.494 61.180 1.00 83.69	С
ATOM	846 C ARG A 412		С
ATOM	847 O ARG A 412	69.998 24.217 63.162 1.00 81.46	0
ATOM		68.604 24.859 60.063 1.00 88.30	С
ATOM		67.453 23.982 60.525 1.00 95.09	С
ATOM		67.522 22.612 59.901 1.00101.21	
ATOM	851 NE ARG A 412	67.033 21.492 60.685 1.00106.04	N
	852 CZ ARG A 412	67.081 20.221 60.269 1.00109.24	С
ATOM	853 NH1 ARG A 412	67.593 19.906 59.082 1.00110.96	N
ATOM	854 NH2 ARG A 412	66.610 19.256 61.058 1.00110.83	N
ATOM	855 N ASN A 413	71.187 23.790 61.345 1.00 86.77	N
ATOM	856 CA ASN A 413	71.997 22.750 61.947 1.00 88.40	С
ATOM		72,726 23.186 63.197 1.00 86.70	С
ATOM	858 O ASN A 413	72.770 22.446 64.194 1.00 84.78	0
ATOM	859 CB ASN A 413	73.003 22.181 60.930 1.00 94.30	С
ATOM	860 CG ASN A 413	73.815 21.042 61.513 1.00 98.85	С
ATOM	861 OD1 ASN A 413	73.568 20.563 62.622 1.00102.19	0
ATOM	862 ND2 ASN A 413	74,833 20.518 60.837 1.00101.25	N
ATOM	863 N GLN A 414	73.361 24.370 63.167 1.00 85.09	N
ATOM	864 CA GLN A 414	73.997 24.886 64.392 1.00 82.79	С
ATOM		72.984 25.035 65.518 1.00 81.33	С
ATOM	866 O GLN A 414	73.180 24.679 66.682 1.00 79.48	Ο
ATOM	867 CB GLN A 414	74.664 26.220 64.092 1.00 81.91	С
ATOM	868 CG GLN A 414	76.063 26.114 63.538 1.00 82.77	С
ATOM		76.431 27.257 62.620 1.00 84.68	С
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0 75.687 27.652 61.712 1.00 85.74 870 OE1 GLN A 414 **ATOM** 77.608 27.859 62.821 1.00 85.01 N 871 NE2 GLN A 414 **ATOM** 71.781 25.527 65.216 1.00 80.63 N 872 N GLY A 415 ATOM 70.742 25.696 66.201 1.00 83.40 C 873 CA GLY A 415 ATOM C 70.340 24.445 66.944 1.00 83.82 874 C GLY A 415 **ATOM** 69.712 24.503 68.003 1.00 84.09 0 875 O GLY A 415 ATOM N 70.653 23.278 66.432 1.00 86.07 876 N LYS A 416 **ATOM** C 70.358 21.991 67.041 1.00 88.46 877 CA LYS A 416 ATOM C 71.346 21.617 68.133 1.00 90.69 878 C LYS A 416 **ATOM** 0 71.114 20.736 68.976 1.00 90.97 879 O LYS A 416 ATOM 70.292 20.922 65.936 1.00 86.72 C 880 CB LYS A 416 ATOM 72.472 22.326 68.256 1.00 92.64 N 885 N CYS A 417 ATOM 73.483 22.108 69.272 1.00 93.07 C 886 CA CYS A 417 ATOM 72.909 22.354 70.666 1.00 93.38 C 887 C CYS A 417 ATOM 0 73.434 21.863 71.658 1.00 92.91 888 O CYS A 417 ATOM 74.701 22.998 69.048 1.00 94.33 C 889 CB CYS A 417 ATOM S 75.678 22.635 67.566 1.00 99.02 890 SG CYS A 417 ATOM N 71.834 23.132 70.752 1.00 93.78 891 N VAL A 418 ATOM C 71.120 23.402 71.968 1.00 93.62 892 CA VAL A 418 ATOM C 69.808 22.596 72.013 1.00 93.64 893 C VAL A 418 ATOM 69.181 22.351 70.999 1.00 91.80 0 894 O VAL A 418 ATOM 70.736 24.892 72.107 1.00 93.31 C 895 CB VAL A 418 ATOM 70.086 25.187 73.456 1.00 91.67 C 896 CG1 VAL A 418 ATOM 71.979 25.742 71.931 1.00 94.17 C 897 CG2 VAL A 418 ATOM 69.412 22.265 73.215 1.00 95.05 N 898 N GLU A 419 ATOM 68.188 21.657 73.643 1.00 95.54 C 899 CA GLU A 419 ATOM 66.973 22.239 72.923 1.00 95.38 C 900 C GLU A 419 ATOM 66.476 23.327 73.242 1.00 95.98 0 901 O GLU A 419 ATOM 67.991 21.962 75.166 1.00 95.46 C 902 CB GLU A 419 ATOM N 66.498 21.521 71.918 1.00 94.14 907 N GLY A 420 ATOM C 65.357 21.884 71.143 1.00 92.12 908 CA GLY A 420 **ATOM** C 65.092 23.320 70.781 1.00 89.03 909 C GLY A 420 **ATOM** 0 64.020 23.850 71.107 1.00 88.17 910 O GLY A 420 ATOM 66.033 23.982 70.089 1.00 86.43 N 911 N MET A 421 **ATOM** C 65.784 25.373 69.683 1.00 82.99 912 CA MET A 421 ATOM C 65,464 25,306 68,175 1,00 80,42 913 C MET A 421 **ATOM** 64.989 26.266 67.583 1.00 80.10 0 914 O MET A 421 **ATOM** C 66.764 26.427 70.019 1.00 81.48 915 CB MET A 421 **ATOM** C 68,244 26,357 69,911 1.00 79.85 916 CG MET A 421 **ATOM** S 69.040 27.989 69.709 1.00 77.79 917 SD MET A 421 **ATOM** 68.655 28.724 71.288 1.00 79.07 C 918 CE MET A 421 **ATOM** 65.609 24.092 67.625 1.00 76.08 N 919 N VAL A 422 **ATOM** C 65.334 23.826 66.229 1.00 71.68 920 CA VAL A 422 **ATOM** C 63.966 24.412 65.856 1.00 67.41 921 C VAL A 422 ATOM 63.776 25.123 64.899 1.00 67.37 0 922 O VAL A 422 ATOM С 65.173 22.322 65.867 1.00 72.40 923 CB VAL A 422 ATOM C 65.967 22.025 64.609 1.00 71.96 924 CG1 VAL A 422 ATOM C 65.512 21.394 67.006 1.00 73.60 925 CG2 VAL A 422 ATOM N 63.017 24.009 66.669 1.00 64.30 926 N GLU A 423 ATOM

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61.623 24.390 66.564 1.00 62.34 C 927 CA GLU A 423 ATOM C 61.457 25.875 66.421 1.00 56.63 **ATOM** 928 C GLU A 423 60.835 26.342 65.468 1.00 54.37 O **ATOM** 929 O GLU A 423 C 60.987 23.849 67.865 1.00 68.72 930 CB GLU A 423 ATOM C 61.513 22.419 68.085 1.00 76.48 931 CG GLU A 423 ATOM 932 CD GLU A 423 61.053 21.478 66.981 1.00 83.18 C ATOM 0 933 OE1 GLU A 423 61.030 21.792 65.757 1.00 84.19 ATOM 60.693 20.332 67.375 1.00 87.12 0 934 OE2 GLU A 423 ATOM 62.064 26.591 67.362 1.00 50.66 935 N ILE A 424 N ATOM 62.014 28.050 67.353 1.00 49.94 C 936 CA ILE A 424 ATOM 62.833 28.671 66.258 1.00 49.72 C 937 C ILE A 424 **ATOM** 938 O ILE A 424 62.454 29.564 65.483 1.00 47.07 O ATOM 62,365 28.585 68.734 1.00 49.44 939 CB ILE A 424 ATOM 940 CG1 ILE A 424 61.957 27.488 69.748 1.00 47.25 C ATOM C 61.546 29.853 68.939 1.00 52.10 941 CG2 ILE A 424 ATOM 61.539 28.004 71.086 1.00 46.42 C 942 CD1 ILE A 424 ATOM 64.032 28.110 66.119 1.00 48.71 N ATOM 943 N PHE A 425 C 64.956 28.558 65.078 1.00 48.83 944 CA PHE A 425 ATOM 64.259 28.554 63.730 1.00 49.83 C ATOM 945 C PHE A 425 64.333 29.486 62.912 1.00 49.75 0 946 O PHE A 425 ATOM C 947 CB PHE A 425 66.079 27.557 65.115 1.00 52.26 ATOM C 67.384 28.056 64.616 1.00 54.82 948 CG PHE A 425 ATOM C 67.534 28.250 63.249 1.00 55.00 949 CD1 PHE A 425 ATOM C 68.429 28.309 65.493 1.00 54.48 950 CD2 PHE A 425 ATOM 68.734 28.713 62.751 1.00 54.74 951 CE1 PHE A 425 ATOM C 69.630 28.763 64.995 1.00 54.33 952 CE2 PHE A 425 ATOM C 69.769 28.957 63.628 1.00 55.26 953 CZ PHE A 425 ATOM 63.592 27.439 63.451 1.00 50.34 N 954 N ASP A 426 ATOM C 62.830 27.302 62.211 1.00 52.02 ATOM 955 CA ASP A 426 61.741 28.379 62.154 1.00 47.88 C 956 C ASP A 426 ATOM 61.620 29.141 61.192 1.00 45.05 957 O ASP A 426 0 ATOM C 62.232 25.927 62.120 1.00 58.40 ATOM 958 CB ASP A 426 C 959 CG ASP A 426 63.114 24.758 61.823 1.00 62.55 ATOM 64.022 24.861 60.962 1.00 65.48 0 ATOM 960 OD1 ASP A 426 62.888 23.686 62.458 1.00 64.32 0 961 OD2 ASP A 426 ATOM 60.978 28.491 63.257 1.00 43.98 N 962 N MET A 427 ATOM 59.955 29.540 63.285 1.00 41.42 C 963 CA MET A 427 ATOM C 964 C MET A 427 60,571 30,896 62,962 1.00 40,52 ATOM 60,206 31.610 62.024 1.00 40.48 0 965 O MET A 427 ATOM C 966 CB MET A 427 59.309 29.529 64.652 1.00 46.35 ATOM C 58.165 28.489 64.737 1.00 48.01 ATOM 967 CG MET A 427 S 57.470 28.508 66.400 1.00 51.78 ATOM 968 SD MET A 427 C 969 CE MET A 427 58.854 28.059 67.403 1.00 45.57 ATOM N 970 N LEUA 428 61.653 31.212 63.699 1.00 37.72 **ATOM** 62.386 32.435 63.480 1.00 36.03 C 971 CA LEU A 428 ATOM 62,778 32.561 62.036 1.00 36.86 C 972 C LEU A 428 **ATOM** 0 973 O LEU A 428 62.648 33.594 61.343 1.00 36.32 ATOM C 974 CB LEU A 428 63.568 32.493 64.467 1.00 36.25 ATOM C 63.098 32.740 65.898 1.00 35.44 975 CG LEU A 428 ATOM

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<b>ATOM</b>	976 CD1 LEU A 428		С
<b>ATOM</b>	977 CD2 LEU A 428	62.723 34.177 66.125 1.00 37.83	С
ATOM	978 N LEU A 429	63.240 31.432 61.475 1.00 40.60	N
<b>ATOM</b>	979 CA LEU A 429	63.706 31.476 60.065 1.00 41.29	С
<b>ATOM</b>	980 C LEU A 429	62.605 31.928 59.145 1.00 39.00	С
<b>ATOM</b>	981 O LEU A 429	62.720 32.870 58.371 1.00 39.51	0
<b>ATOM</b>		64.313 30.144 59.690 1.00 <b>43.2</b> 7	С
<b>ATOM</b>	983 CG LEU A 429	65.812 30.002 59.966 1.00 45.30	С
<b>ATOM</b>	984 CD1 LEU A 429	66.293 28.587 59.649 1.00 45.70	С
<b>ATOM</b>	985 CD2 LEU A 429	66.629 31.027 59.197 1.00 43.74	С
<b>ATOM</b>	986 N ALA A 430	61.448 31.309 59.364 1.00 39.75	N
<b>ATOM</b>	987 CA ALA A 430	60.243 31.583 58.587 1.00 37.09	C
ATOM	988 C ALA A 430	59.798 33.011 58.767 1.00 38.56	С
ATOM	989 O ALA A 430	59.521 33.697 57.752 1.00 38.33	0
ATOM	990 CB ALA A 430	59.208 30.593 59.021 1.00 39.99	C
ATOM	991 N THR A 431	59.882 33.500 60.028 1.00 35.59	N
ATOM		59.549 34.937 60.144 1.00 36.46	С
ATOM	993 C THR A 431	60.428 35.826 59.333 1.00 37.93	С
ATOM	994 O THR A 431	59.934 36.643 58.554 1.00 38.61	0
ATOM	995 CB THR A 431	59.488 35.351 61.600 1.00 36.66	С
ATOM	996 OG1 THR A 431	58.696 34.368 62.308 1.00 44.00	Ο
ATOM			С
ATOM	998 N SER A 432	61.781 35.804 59.328 1.00 43.67	N
ATOM	999 CA SER A 432	62.459 36.829 58.499 1.00 45.86	С
ATOM		62.140 36.599 57.029 1.00 45.06	С
ATOM		62.151 37.499 56.200 1.00 40.01	0
ATOM	1002 CB SER A 432	63.961 37.037 58.613 1.00 45.04	С
ATOM	1003 OG SER A 432	64.652 35.870 58.844 1.00 44.31	Ο
ATOM	1004 N SER A 433	61.942 35.297 56.773 1.00 47.09	N
ATOM		61.611 35.007 55.384 1.00 49.54	С
	1006 C SER A 433	60.360 35.760 54.981 1.00 49.50	С
		60.276 36.385 53.896 1.00 51.37	Ο
		61.533 33.492 55.255 1.00 50.61	С
	1009 OG SER A 433		0
	1010 N ARG A 434	59.359 35.767 55.868 1.00 45.71	N
	1011 CA ARG A 434	58.112 36.442 55.471 1.00 45.67	C
	1012 C ARG A 434	58.365 37.904 55.424 1.00 45.99	С
	1013 O ARG A 434	57.741 38.684 54.686 1.00 48.03	0
	1014 CB ARG A 434	56,994 35.888 56.328 1.00 52.87	С
	1015 CG ARG A 434	55,825 36,768 56,669 1,00 61,64	С
ATOM		54,448 36,253 56,247 1.00 65.66	С
ATOM		53,910 37,123 55,212 1,00 71,37	N
	1018 CZ ARG A 434	52,755 37,777 55,178 1.00 74,32	С
	1019 NH1 ARG A 434	51.884 37.683 56.194 1.00 76.56	N
ATOM			N
	1021 N PHE A 435	59.278 38.400 56.271 1.00 45.66	N
	1022 CA PHE A 435	59.591 39.822 56.251 1.00 46.91	С
ATOM		60.212 40.184 54.893 1.00 44.85	С
ATOM	1024 O PHE A 435	60.006 41.239 54.325 1.00 45.13	Ο
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ATOM	1025	CB PHE A 435	60.586 40.207 57.352 1.00 48.27	С
ATOM		CG PHE A 435	59.982 40.529 58.672 1.00 51.19	С
ATOM		CD1 PHE A 435		С
<b>ATOM</b>		CD2 PHE A 435	60.782 40.922 59.746 1.00 47.96	С
<b>ATOM</b>		CE1 PHE A 435	58.025 40.713 60.097 1.00 52.73	С
<b>ATOM</b>		CE2 PHE A 435	60.194 41.181 60.955 1.00 47.26	С
<b>ATOM</b>		CZ PHE A 435	58.840 41.076 61.157 1.00 48.94	С
<b>ATOM</b>	1032	N ARG A 436	61.056 39.323 54.400 1.00 47.63	N
<b>ATOM</b>			61.746 39.482 53.124 1.00 49.34	C
<b>ATOM</b>	1034	C ARG A 436	60.645 39.474 52.078 1.00 49.53	С
<b>ATOM</b>	1035		60.330 40.477 51.451 1.00 45.06	О
<b>ATOM</b>			62.682 38.315 52.896 1.00 50.60	С
<b>ATOM</b>	1037	CG ARG A 436	63.939 38.648 52.124 1.00 56.76	C
<b>ATOM</b>	1038	CD ARG A 436	64.616 37.327 51.713 1.00 61.86	С
<b>ATOM</b>	1039	NE ARG A 436	65.061 36.607 52.886 1.00 66.94	N
<b>ATOM</b>			64.776 35.363 53.238 1.00 70.98	С
<b>ATOM</b>	1041	NH1 ARG A 436	63.978 34.637 52.445 1.00 72.78	N
<b>ATOM</b>	1042	NH2 ARG A 436	65.262 34.887 54.395 1.00 71.17	N
<b>ATOM</b>	1043	N MET A 437	59.931 38.317 52.119 1.00 53.08	N
<b>ATOM</b>	1044	CA MET A 437	58.819 38.277 51.152 1.00 57.01	С
<b>ATOM</b>	1045	C MET A 437	58.080 39.607 51.214 1.00 55.26	C
<b>ATOM</b>	1046	O MET A 437	58.069 40.283 50.197 1.00 57.39	Ο
<b>ATOM</b>	1047	CB MET A 437	57.941 37.108 51.344 1.00 63.52	,C
<b>ATOM</b>	1048	CG MET A 437	58.313 35.727 50.890 1.00 71.66	С
<b>ATOM</b>	1049	SD MET A 437	57.582 34.534 52.062 1.00 84.11	S
<b>ATOM</b>	1050	CE MET A 437	55.865 35.144 52.090 1.00 79.21	С
<b>ATOM</b>	1051	N MET A 438	57.523 40.091 52.326 1.00 51.51	N
ATOM	1052	CA MET A 438	56.773 41.324 52.297 1.00 51.37	С
<b>ATOM</b>	1053	C MET A 438		C
<b>ATOM</b>	1054	O MET A 438	56.893 43.685 51.973 1.00 48.99	Ο
<b>ATOM</b>			56.028 41.518 53.621 1.00 52.61	С
ATOM	1056	CG MET A 438	55.222 40.334 54.061 1.00 54.98	С
<b>ATOM</b>		SD MET A 438		S
<b>ATOM</b>	1058	CE MET A 438	53.926 42.358 55.466 1.00 55.04	Ç
		N ASN A 439	58.846 42.523 51.964 1.00 48.54	N
		CA ASN A 439	59.767 43.614 51.794 1.00 45.77	С
		C ASN A 439	59.605 44.567 52.968 1.00 42.78	С
<b>ATOM</b>	1062	O ASN A 439	59.522 45.787 52.761 1.00 39.35	О
<b>ATOM</b>		CB ASN A 439	59.622 44.374 50.518 1.00 53.65	С
<b>ATOM</b>		CG ASN A 439	60.859 45.147 50.093 1.00 60.47	С
<b>ATOM</b>	1065	OD1 ASN A 439	61.779 45.547 50.798 1.00 58.68	0
<b>ATOM</b>		ND2 ASN A 439	60.875 45.410 48.768 1.00 65.24	N
<b>ATOM</b>	1067	N LEU A 440	59.545 43.937 54.172 1.00 39.68	N
ATOM		CA LEU A 440	59.363 44.798 55.341 1.00 40.85	С
		C LEU A 440	60.302 45.992 55.289 1.00 40.66	С
		O LEU A 440	61.439 45.917 54.837 1.00 40.49	0
ATOM		CB LEU A 440	59.506 44.052 56.677 1.00 42.20	C
ATOM		CG LEU A 440	59.201 45.057 57.839 1.00 43.75	С
ATOM	1073	CD1 LEU A 440	57.802 45.601 57.642 1.00 45.00	С

ATOM 1074 CD2 LEU A 440 59.380 44.431 59.202 1.00 42.76 C N 59.881 47.156 55.736 1.00 42.17 ATOM 1075 N GLN A 441 60.755 48.326 55.684 1.00 42.54 C ATOM 1076 CA GLN A 441 C 61.111 48.837 57.064 1.00 45.77 ATOM 1077 C GLN A 441 0 ATOM 1078 O GLN A 441 60.289 48.917 57.992 1.00 46.95 ATOM 1079 CB GLN A 441 59.947 49.392 54.913 1.00 44.80 C 59.648 48.869 53.469 1.00 46.60 ATOM 1080 CG GLN A 441 60.870 49.261 52.620 1.00 46.29 ATOM 1081 CD GLN A 441 ATOM 1082 OE1 GLN A 441 61.209 50.473 52.644 1.00 43.94 61.391 48.217 51.988 1.00 43.50 N ATOM 1083 NE2 GLN A 441 62.361 49.221 57.240 1.00 44.76 ATOM 1084 N GLY A 442 N ATOM 1085 CA GLY A 442 62,942 49,758 58,436 1,00 41,75 C 61.971 50.542 59.255 1.00 41.41 C ATOM 1086 C GLY A 442 ATOM 1087 O GLY A 442 61.661 50.119 60.370 1.00 43.47 0 61.418 51.600 58.688 1.00 43.44 ATOM 1088 N GLU A 443 ATOM 1089 CA GLU A 443 60.442 52.464 59.287 1.00 43.18 C ATOM 1090 C GLU A 443 59.181 51.714 59.768 1.00 41.51 C ATOM 1091 O GLU A 443 58.536 52.266 60.688 1.00 41.33 ATOM 1092 CB GLU A 443 60.005 53.585 58.352 1.00 45.30 ATOM 1093 CG GLU A 443 60.996 54.545 57.786 1.00 46.12 C 61.854 53.906 56.720 1.00 51.40 ATOM 1094 CD GLU A 443 61.523 52.818 56.225 1.00 51.51 0 ATOM 1095 OE1 GLU A 443 ATOM 1096 OE2 GLU A 443 62.932 54.443 56.343 1.00 57.58 - 0 ATOM 1097 N GLU A 444 58.830 50.580 59.194 1.00 37.35 N ATOM 1098 CA GLU A 444 57.661 49.801 59.612 1.00 38.11 C 58.071 48.899 60.782 1.00 36.47 ATOM 1099 C GLU A 444 ATOM 1100 O GLU A 444 57.364 48.667 61.760 1.00 40.60 0 ATOM 1101 CB GLU A 444 57.126 48.855 58.543 1.00 40.40 C ATOM 1102 CG GLU A 444 56.654 49.456 57.251 1.00 43.75 ATOM 1103 CD GLU A 444 56.171 48.486 56.187 1.00 44.27 56.948 47.714 55.593 1.00 42.90 0 ATOM 1104 OE1 GLU A 444 ATOM 1105 OE2 GLU A 444 54,945 48.547 55.928 1.00 43.73 0 ATOM 1106 N PHE A 445 59.274 48.392 60.688 1.00 36.90 N ATOM 1107 CA PHE A 445 59.910 47.530 61.676 1.00 36.32 C 59.990 48.218 63.020 1.00 38.08 C ATOM 1108 C PHE A 445 ATOM 1109 O PHE A 445 59.624 47.708 64.078 1.00 43.18 O ATOM 1110 CB PHE A 445 61.324 47.215 61.222 1.00 33.88 C 62.219 46.649 62.240 1.00 34.44 ATOM 1111 CG PHE A 445 ATOM 1112 CD1 PHE A 445 62.075 45.370 62.709 1.00 33.30 C C 63.265 47.438 62.742 1.00 35.81 ATOM 1113 CD2 PHE A 445 ATOM 1114 CE1 PHE A 445 62.975 44.855 63.646 1.00 35.64 C ATOM 1115 CE2 PHE A 445 64.199 46.911 63.618 1.00 34.03 C C 64.031 45.624 64.090 1.00 33.63 ATOM 1116 CZ PHE A 445 ATOM 1117 N VAL A 446 60.370 49.468 62.998 1.00 36.38 N C ATOM 1118 CA VAL A 446 60.501 50.229 64.260 1.00 35.39 59.160 50.513 64.836 1.00 36.39 C ATOM 1119 C VAL A 446 58.899 50.721 66.060 1.00 36.88 ATOM 1120 O VAL A 446 0 ATOM 1121 CB VAL A 446 61.340 51.422 63.743 1.00 37.96 C ATOM 1122 CG1 VAL A 446 61.016 52.732 64.350 1.00 36.13 C

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ATOM	1123 CG2 VAL A 446	62.806 51.032 63.810 1.00 36.84	С
ATOM	1124 N CYS A 447	58.166 50.587 63.959 1.00 38.09	N
ATOM	1125 CA CYS A 447	56.756 50.836 64.384 1.00 36.81	С
ATOM	1126 C CYS A 447	56.242 49.584 65.066 1.00 35.90	С
ATOM	1127 O CYS A 447	55.686 49.628 66.147 1.00 36.40	Ο
ATOM	1128 CB CYS A 447	56.001 51.134 63.134 1.00 39.05	С
ATOM	1129 SG CYS A 447	55.897 52.861 62.706 1.00 45.24	S
ATOM	1130 N LEU A 448	56.515 48.431 64.448 1.00 37.34	N
ATOM	1131 CA LEU A 448	56.179 47.116 65.016 1.00 36.19	С
ATOM	1132 C LEU A 448	56.884 46.877 66.333 1.00 35.93	С
ATOM	1133 O LEU A 448	56,332 46,318 67,303 1,00 36,91	Ο
ATOM	1134 CB LEU A 448	56,644 46,016 64,059 1.00 37,42	С
ATOM	1135 CG LEU A 448	55.919 45.875 62.723 1.00 38.60	С
ATOM	1136 CD1 LEU A 448	56,204 44,485 62,166 1,00 38,61	С
ATOM	1137 CD2 LEU A 448	54.407 46.000 62.875 1.00 38.37	С
ATOM	1138 N LYS A 449	58,161 47,327 66,475 1.00 34.08	N
ATOM	1139 CA LYS A 449	58.759 47.056 67.800 1.00 33.35	С
ATOM	1140 C LYS A 449	58.051 47.861 68.885 1.00 32.12	С
ATOM	1141 O LYS A 449	57.772 47.421 69.977 1.00 31.98	Ο
ATOM	1142 CB LYS A 449	60.222 47.413 67.867 1.00 35.64	С
ATOM		61.196 46.311 67.540 1.00 40.11	С
ATOM		62.593 46.562 68.113 1.00 37.82	С
ATOM	1145 CE LYS A 449	63.209 47.746 67.359 1.00 39.59	С
ATOM	1146 NZ LYS A 449	64.552 48.079 67.932 1.00 45.13	N
ATOM	1147 N SER A 450	57.796 49.148 68.608 1.00 32.09	N
<b>ATOM</b>	1148 CA SER A 450	57.214 49.985 69.643 1.00 32.69	С
<b>ATOM</b>	1149 C SER A 450	55.872 49.379 70.046 1.00 35.21	С
<b>ATOM</b>	1150 O SER A 450	55.572 49.405 71.237 1.00 35.15	0_
<b>ATOM</b>	1151 CB SER A 450	57.093 51.427 69.253 1.00 33.33	C
<b>ATOM</b>		58.301 51.920 68.712 1.00 44.51	0
<b>ATOM</b>	1153 N ILE A 451	55.152 48.892 69.015 1.00 31.47	N
<b>ATOM</b>	1154 CA ILE A 451	53.871 48.281 69.300 1.00 29.67	С
	1155 C ILE A 451		C
	1156 O ILE A 451	53.319 46.948 71.179 1.00 30.52	0
ATOM	1157 CB ILE A 451	53.185 47.857 67.987 1.00 30.16	C
ATOM		52.654 49.104 67.276 1.00 29.31	C
ATOM		52.097 46.805 68.217 1.00 25.93	C
ATOM	1160 CD1 ILE A 451	52.274 48.796 65.821 1.00 32.04	C
ATOM		55.075 46.229 69.918 1.00 28.54	N
ATOM		55.300 45.060 70.761 1.00 25.63	C
ATOM	1163 C ILE A 452	55.576 45.545 72.180 1.00 30.38	С
	1164 O ILE A 452	55.079 45.005 73.137 1.00 34.58	0
	1165 CB ILE A 452	56.469 44.234 70.281 1.00 26.82	C
ATOM		56.170 43.518 68.957 1.00 30.90	C
ATOM		57.009 43.259 71.314 1.00 21.12	C C
ATOM		57.349 42.688 68.405 1.00 25.51	N
ATOM		56.367 46.581 72.361 1.00 32.06	C
ATOM		56.675 47.098 73.654 1.00 34.04	c
ATOM	1171 C LEU A 453	55.436 47.537 74.371 1.00 34.53	C

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			55/3
TOM	1172	O LEU A 453	55.177 47
TOM	1173	CB LEU A 453	57.676 48

O 1.100 75.495 1.00 40.58 A. C 8.265 73.594 1.00 33.55 A. 57.973 48.870 74.984 1.00 31.37 C ATOM 1174 CG LEU A 453 58.292 47.746 75.949 1.00 27.35 C ATOM 1175 CD1 LEU A 453 58,980 49,992 74,961 1.00 26.50 C ATOM 1176 CD2 LEU A 453 54.627 48.386 73.806 1.00 35.04 N ATOM 1177 N LEU A 454 C 53.404 48.815 74.482 1.00 35.08 ATOM 1178 CA LEU A 454 52.313 47.814 74.641 1.00 37.41 C ATOM 1179 C LEU A 454 ATOM 1180 O LEU A 454 51.468 47.943 75.510 1.00 36.19 0 52.775 49.973 73.645 1.00 32.94 C ATOM 1181 CB LEU A 454 53,728 51.185 73.576 1.00 34.24 C ATOM 1182 CG LEU A 454 C ATOM 1183 CD1 LEU A 454 53.055 52.297 72.825 1.00 32.61 54.126 51.597 74.987 1.00 34.42 C ATOM 1184 CD2 LEU A 454 ATOM 1185 N ASN A 455 52.180 46.850 73.728 1.00 42.96 N C 51.060 45.936 73.771 1.00 44.63 ATOM 1186 CA ASN A 455 C ATOM 1187 C ASN A 455 51,238 44,638 74,476 1,00 47.81 ATOM 1188 O ASN A 455 50.303 44.023 74.961 1.00 52.94 0 C 50.762 45.569 72.292 1.00 44.66 ATOM 1189 CB ASN A 455 49,596 44,620 72,164 1.00 43,46 C ATOM 1190 CG ASN A 455 0 ATOM 1191 OD1 ASN A 455 49.696 43.551 71.583 1.00 42.54 48,475 45.034 72.727 1.00 46.97 N ATOM 1192 ND2 ASN A 455 52.395 44.046 74.548 1.00 50.76 N ATOM 1193 N SER A 456 52.427 42.713 75.145 1.00 53.37 C ATOM 1194 CA SER A 456 C ATOM 1195 C SER A 456 52.032 42.695 76.583 1.00 56.18 51.549 41.691 77.113 1.00 56.74 0 ATOM 1196 O SER A 456 53.794 42.093 74.786 1.00 52.37 C ATOM 1197 CB SER A 456 53.964 41.972 73.368 1.00 40.19 0 ATOM 1198 OG SER A 456 52.241 43.761 77.316 1.00 61.86 N ATOM 1199 N GLY A 457 51.997 43.862 78.731 1.00 70.54 C ATOM 1200 CA GLY A 457 C 50.833 44.726 79.116 1.00 77.77 ATOM 1201 C GLY A 457 50.450 44.776 80.284 1.00 78.76 0 ATOM 1202 O GLY A 457 N 50.151 45.356 78.171 1.00 84.38 ATOM 1203 N VAL A 458 ATOM 1204 CA VAL A 458 48.987 46.195 78.378 1.00 90.25 C C ATOM 1205 C VAL A 458 47.897 45.551 79.210 1.00 96.24 O 46,948 46.250 79.609 1.00 98.11 ATOM 1206 O VAL A 458 C ATOM 1207 CB VAL A 458 48.448 46.636 76.990 1.00 89.27 47,739 45,491 76,289 1,00 89,46 C ATOM 1208 CG1 VAL A 458 C ATOM 1209 CG2 VAL A 458 47.547 47.845 77.079 1.00 88.97 N 47.924 44.257 79.513 1.00101.74 ATOM 1210 N TYR A 459 46.973 43.497 80.269 1.00104.80 C ATOM 1211 CA TYR A 459 C ATOM 1212 C TYR A 459 47.332 43.286 81.740 1.00105.22 0 ATOM 1213 O TYR A 459 47.016 42.180 82.231 1.00105.07 46.814 42.080 79.662 1.00107.02 C ATOM 1214 CB TYR A 459 45.822 42.038 78.519 1.00110.17 ATOM 1215 CG TYR A 459 45.419 43.212 77.893 1.00110.98 C ATOM 1216 CD1 TYR A 459 C ATOM 1217 CD2 TYR A 459 45.308 40.830 78.053 1.00110.39 C 44.545 43.205 76.835 1.00112.30 ATOM 1218 CE1 TYR A 459 44.418 40.816 76.997 1.00112.11 C ATOM 1219 CE2 TYR A 459 C 44.051 42.000 76.399 1.00112.88 ATOM 1220 CZ TYR A 459

42 160 41 001 75 347 1 00115 80	Ο
43.168 41.991 75.547 1.00115.00	N
42.526.57.004.82.435.1.00107.02	C
44.900 56.630 91.840 1.00107.02	c
45.262.57.200.90.043.1.00105.40	Ö
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	C
45.728 53.170 81.002 1.00 95.72	N
45.352 52.182 79.990 1.00 88.76	С
	C
	0
	С
	N
44.142 53.947 78.917 0.50 81.68	N
43.735 54.858 77.861 0.50 76.63	С
43.727 54.830 77.848 0.50 78.99	С
	C
44.863 55.585 77.186 0.50 74.62	С
44.906 55.645 75.937 0.50 70.54	О
45.017 55.398 75.961 0.50 73.32	Ο
42.788 55.917 78.446 0.50 77.43	С
	С
	С
	С
	O
	0
	C
	C
	N
47 039 56 684 77.314 1.00 64.59	C
47 754 55 773 76.335 1.00 60.83	С
	0
48 007 57 255 78 327 1.00 64.63	С
49 247 57 893 77.753 1.00 66.15	С
	N
50 560 57 566 77 949 1.00 63.36	С
50.461 59.305 76.567 1.00.63.50	С
51 263 58 458 77 202 1 00 64 89	N
49.085.54.566.76.816.1.00.56.86	N
49.702 52.658 75.933 1.00.56.72	C
	c
40.013 33.321 14.001 1.00 31.11 40.606 52.220 72 567 1.00 54.05	Ö
40.000 33.220 /3.30/ 1.00 37.03	C
	C
	C
50.144 51.632 /5.633 1.00 60.22	C
	44.142 53.947 78.917 0.50 81.68 43.735 54.858 77.861 0.50 76.63 43.727 54.830 77.848 0.50 78.99 44.905 55.533 77.166 0.50 72.53

ATON (	1282 CD1 ILE A 475	50.468 51.438 78.616 1.00 63.03	С
ATOM		46.701 53.150 74.800 1.00 55.97	N
ATOM	1284 CA HIS A 476	45.863 52.867 73.648 1.00 58.59	С
ATOM ATOM	1285 C HIS A 476	45.863 53.976 72.617 1.00 59.35	С
	1286 O HIS A 476	45.714 53.730 71.394 1.00 61.12	0
ATOM	1287 CB HIS A 476	44.463 52.526 74.106 1.00 64.75	С
ATOM	1288 CG HIS A 476		С
ATOM	1289 ND1 HIS A 476	45.206 50.100 74.365 1.00 73.22	N
ATOM	1290 CD2 HIS A 476	43.393 50.595 75.501 1.00 74.42	С
ATOM	1291 CE1 HIS A 476		Č
ATOM	1292 NE2 HIS A 476	43.721 49.266 75.694 1.00 74.59	N
ATOM	1293 N ARG A 477	46.135 55.219 73.001 1.00 58.21	N
ATOM	1294 CA ARG A 477	46.136 56.304 72.015 1.00 57.66	C
ATOM		47.505 56.399 71.380 1.00 55.49	C
ATOM	1295 C ARG A 477 1296 O ARG A 477		Ö
ATOM	1297 CB ARG A 477		Ċ
ATOM	-	44.852 57.527 73.864 1.00 66.35	Č
ATOM	1298 CG ARG A 477	43.749 58.567 73.887 1.00 69.29	č
ATOM	1299 CD ARG A 477	44.206 59.875 73.400 1.00 72.49	N
ATOM	1300 NE ARG A 477	44.206 39.873 73.400 1.00 72.43 48.506 55.917 72.109 1.00 51.61	N
ATOM	1304 N VAL A 478	49.864 55.952 71.511 1.00 48.31	Ċ
ATOM	1305 CA VAL A 478	49.873 54.851 70.465 1.00 45.77	c
ATOM	1306 C VAL A 478		o ·
ATOM	1307 O VAL A 478		Č
ATOM	1308 CB VAL A 478	52.313 55.702 71.995 1.00 47.97	C
ATOM	1309 CG1 VAL A 478		č
ATOM	1310 CG2 VAL A 478	49.226 53.747 70.861 1.00 44.03	N
ATOM	1311 N LEU A 479	49.088 52.587 69.976 1.00 41.04	Ĉ
ATOM	1312 CA LEU A 479	49.088 32.387 69.976 1.00 41.04	c
ATOM	1313 C LEU A 479		Ö
ATOM	1314 O LEU A 479		. C
ATOM	1315 CB LEU A 479		C
ATOM		49.306 50.514 71.497 1.00 41.14 48.428 49.487 72.159 1.00 38.92	Č
ATOM	1317 CD1 LEU A 479	50.463 49.928 70.690 1.00 36.46	č
	1318 CD2 LEU A 479	47.211 53.712 68.960 1.00 42.05	N
	1319 N ASP A 480		Ĉ
	1320 CA ASP A 480	47.374 55.147 66.986 1.00 42.83	c
	1321 C ASP A 480	47.305 55.139 65.748 1.00 42.30	Ö
	1322 O ASP A 480	45.201 54.953 68.099 1.00 42.23	C
	1323 CB ASP A 480	43.201 34.933 68.099 1.00 42.23	č
ATOM	1324 CG ASP A 480	43.932 52.968 68.567 1.00 42.99	o
	1325 OD1 ASP A 480		Ö
	1326 OD2 ASP A 480	43.187 54.890 69.284 1.00 48.06	N
	1327 N LYS A 481	48.194 55.938 67.729 1.00 41.96	C
	1328 CA LYS A 481	49.063 56.824 66.929 1.00 44.36	c
	1329 C LYS A 481	50.015 55.990 66.111 1.00 39.42	o
	1330 O LYS A 481	50.178 56.356 64.967 1.00 40.40	C
ATOM		49.767 57.875 67.765 1.00 50.78	C
	1332 CG LYS A 481		C
ATOM	1333 CD LYS A 481	50.362 60.262 67.571 1.00 59.84	C

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ATOM	1334		50.299 61.305 66.443 1.00 64.03	С
ATOM	1335	NZ LYS A 481	48.891 61.472 65.919 1.00 65.06	N
ATOM	1336	N ILE A 482	50.585 54.906 66.617 1.00 37.30	N
ATOM	1337	CA ILE A 482	51.484 54.115 65.740 1.00 37.67	С
<b>ATOM</b>	1338	C ILE A 482	50.784 53.474 64.576 1.00 37.39	C
ATOM	1339	O ILE A 482	51.369 53.361 63.504 1.00 40.01	Ο
ATOM	1340	CB ILE A 482	52.223 53.033 66.573 1.00 38.51	С
ATOM	1341	CG1 ILE A 482	52.717 53.713 67.841 1.00 37.12	C
<b>ATOM</b>	1342	CG2 ILE A 482	53.229 52.354 65.681 1.00 32.84	C
<b>ATOM</b>	1343	CD1 ILE A 482	53.464 52.910 68.842 1.00 36.63	С
<b>ATOM</b>	1344	N THR A 483	49.541 53.024 64.688 1.00 37.56	N
<b>ATOM</b>	1345	CA THR A 483	48.801 52.521 63.553 1.00 38.49	С
<b>ATOM</b>	1346	C THR A 483	48.707 53.631 62.498 1.00 41.74	С
<b>ATOM</b>	1347	O THR A 483	49.115 53.398 61.323 1.00 41.89	О
<b>ATOM</b>	1348	CB THR A 483	47.358 52.105 63.878 1.00 39.30	С
<b>ATOM</b>	1349	OG1 THR A 483	47.465 50.929 64.705 1.00 40.84	0
<b>ATOM</b>	1350	CG2 THR A 483	46.655 51.747 62.564 1.00 36.88	С
<b>ATOM</b>	1351	N ASP A 484	48.231 54.813 62.941 1.00 43.21	N
<b>ATOM</b>	1352	CA ASP A 484	48.226 55.987 62.034 1.00 43.09	С
<b>ATOM</b>	1353	C ASP A 484	49.567 56.088 61.303 1.00 42.19	С
<b>ATOM</b>	1354	O ASP A 484	49.591 56.087 60.048 1.00 43.92	0
<b>ATOM</b>	1355	CB ASP A 484	48.063 57.317 62.737 1.00 43.77	С
<b>ATOM</b>	1356	CG ASP A 484	46.749 57.475 63.456 1.00 47.64	С
<b>ATOM</b>	1357	OD1 ASP A 484	45.800 56.705 63.146 1.00 46.18	0
<b>ATOM</b>	1358	OD2 ASP A 484	46.681 58.362 64.347 1.00 51.47	Q
<b>ATOM</b>	1359	N THR A 485	50.645 56.123 62.071 1.00 39.45	N
<b>ATOM</b>	1360	CA THR A 485	51.990 56.225 61.436 1.00 40.57	С
<b>ATOM</b>	1361	C THR A 485	52.253 55.079 60.500 1.00 40.59	С
<b>ATOM</b>	1362	O THR A 485	52.717 55.274 59.365 1.00 44.93	0
<b>ATOM</b>		CB THR A 485		С
<b>ATOM</b>	1364	OG1 THR A 485	52.575 56.995 63.625 1.00 35.82	О
<b>ATOM</b>	1365	CG2 THR A 485	54.377 56.779 61.950 1.00 34.78	С
<b>ATOM</b>	1366	N LEU A 486	51.912 53.873 60.902 1.00 42.16	N
ATOM	1367	CA LEU A 486	52.127 52.729 59.939 1.00 43.09	С
ATOM	1368	C LEU A 486	51.312 52.966 58.681 1.00 40.80	С
		O LEU A 486		Ο
		CB LEU A 486	51.755 51.499 60.688 1.00 42.99	С
		CG LEU A 486		С
			54.082 50.478 60.590 1.00 44.10	С
ATOM	1373	CD2 LEU A 486		С
		N ILE A 487	50.040 53.365 58.786 1.00 42.87	N
		CA ILE A 487	49.240 53.582 57.545 1.00 44.76	С
<b>ATOM</b>	1376	C ILE A 487	49.755 54.772 56.749 1.00 44.95	С
		O ILE A 487		0
		CB ILE A 487	47.760 53.764 57.879 1.00 45.98	С
		CG1 ILE A 487	47.046 52.483 58.286 1.00 42.68	С
		CG2 ILE A 487	47.016 54.425 56.725 1.00 48.28	C
		CD1 ILE A 487	47.114 51.396 57.264 1.00 43.54	С
ATOM	1382	N HIS A 488	50.166 55.842 57.432 1.00 48.83	N

<b>ATOM</b>	1383 CA HIS A 488	50.832 56.961 56.775 1.00 49.75	С
<b>ATOM</b>	1384 C HIS A 488	52.052 56.545 55.987 1.00 48.04	С
<b>ATOM</b>	1385 O HIS A 488	52.308 57.018 54.876 1.00 52.94	Ο
<b>ATOM</b>	1386 CB HIS A 488	51.218 57.976 57.860 1.00 52.56	С
ATOM	1387 CG HIS A 488	51.999 59.098 57.240 1.00 57.68	С
ATOM	1388 ND1 HIS A 488	53.327 58.970 56.882 1.00 59.10	N
ATOM	1389 CD2 HIS A 488	51.620 60.355 56.920 1.00 59.02	С
ATOM	1390 CE1 HIS A 488	53.745 60.115 56.366 1.00 59.80	С
ATOM	1391 NE2 HIS A 488	52.734 60.958 56.385 1.00 60.71	N
ATOM	1392 N LEU A 489	52.888 55.639 56.452 1.00 46.72	N
ATOM	1393 CA LEU A 489	54.044 55.192 55.690 1.00 45.24	С
ATOM	1394 C LEU A 489	53.585 54.449 54.440 1.00 44.92	С
<b>ATOM</b>	1395 O LEU A 489	54.325 54.409 53.459 1.00 46.98	0
<b>ATOM</b>	1396 CB LEU A 489	54.900 54.199 56.516 1.00 44.02	С
<b>ATOM</b>	1397 CG LEU A 489	55.743 54.841 57.628 1.00 46.75	С
<b>ATOM</b>	1398 CD1 LEU A 489	56.068 53.856 58.738 1.00 45.91	С
<b>ATOM</b>	1399 CD2 LEU A 489	57.037 55.400 57.046 1.00 43.69	C
<b>ATOM</b>	1400 N MET A 490	52.442 53.798 54.508 1.00 44.91	N
ATOM	1401 CA MET A 490	51.965 52.951 53.418 1.00 48.26	С
ATOM	1402 C MET A 490	51.365 53.704 52.253 1.00 48.02	С
ATOM	1403 O MET A 490	51.571 53.374 51.069 1.00 43.52	Ο
ATOM	1404 CB MET A 490	50.931 51.977 54.030 1.00 51.41	С
ATOM		51.672 50.853 54.797 1.00 49.69	C
	1406 SD MET A 490	50.415 49.777 55.481 1.00 47.26	S
	1407 CE MET A 490		С
ATOM	1408 N ALA A 491	50.596 54.711 52.631 1.00 50.20	N
ATOM	1409 CA ALA A 491	49.971 55.677 51.736 1.00 52.27	C
ATOM	1410 C ALA A 491	51.094 56.449 51.046 1.00 57.27	С
<b>ATOM</b>	1411 O ALA A 491	51.364 56.361 49.852 1.00 57.13	0
<b>ATOM</b>	1412 CB ALA A 491	49.144 56.667 52.566 1.00 50.19	С
<b>ATOM</b>	1413 N LYS A 492	51.947 57.103 51.868 1.00 60.59	N
ATOM	1414 CA LYS A 492		Ċ.
	1415 C LYS A 492	53.843 56.912 50.319 1.00 61.77	С
<b>ATOM</b>	1416 O LYS A 492	54.478 57.443 49.416 1.00 63.72	0
<b>ATOM</b>	1417 CB LYS A 492	53.920 58.444 52.351 1.00 63.55	С
<b>ATOM</b>	1418 CG LYS A 492		С
<b>ATOM</b>	1422 N ALA A 493		N
<b>ATOM</b>	1423 CA ALA A 493		С
<b>ATOM</b>	1424 C ALA A 493	53.686 54.393 48.342 1.00 61.29	C
<b>ATOM</b>	1425 O ALA A 493	54.118 53.636 47.472 1.00 60.89	0
<b>ATOM</b>	1426 CB ALA A 493	54.964 53.443 50.284 1.00 58.60	С
<b>ATOM</b>	1427 N GLY A 494	52.464 54.897 48.330 1.00 61.59	N
<b>ATOM</b>	1428 CA GLY A 494	51.542 54.710 47.240 1.00 63.74	С
ATOM	1429 C GLY A 494	50.555 53.594 47.368 1.00 65.33	С
<b>ATOM</b>	1430 O GLY A 494		0
	1431 N LEU A 495		N
ATOM	1432 CA LEU A 495		С
ATOM		48.134 52.271 48.443 1.00 58.06	С
ATOM	1434 O LEU A 495	47.735 53.379 48.799 1.00 56.91	0
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ATOM	1435	CB LEU A 495	49.732 51.021 49.907 1.00 58.36	С
ATOM	1436	CG LEU A 495	50.979 50.136 50.029 1.00 57.55	С
<b>ATOM</b>	1437	CD1 LEU A 495	50.646 48.750 50.538 1.00 52.48	С
<b>ATOM</b>	1438	CD2 LEU A 495	51.767 50.006 48.718 1.00 58.19	C
ATOM	1439	N THR A 496	47.275 51.380 47.919 1.00 58.45	N
ATOM	1440	CA THR A 496	45.857 51.787 47.808 1.00 57.29	С
ATOM	1441	C THR A 496	45.259 51.746 49.201 1.00 55.11	C
ATOM	1442	O THR A 496	45.842 51.087 50.052 1.00 57.18	0
<b>ATOM</b>	1443	CB THR A 496	45.038 50.909 46.867 1.00 57.90	С
ATOM	1444	OG1 THR A 496	44.908 49.584 47.382 1.00 59.37	0
ATOM	1445	CG2 THR A 496	45.608 50.827 45.465 1.00 55.46	С
ATOM	1446	N LEU A 497	44.128 52.356 49.468 1.00 55.27	N
ATOM		CA LEU A 497	43.533 52.264 50.784 1.00 57.86	С
ATOM	1448	C LEU A 497	43.296 50.776 51.100 1.00 58.92	С
ATOM	1449	O LEU A 497	43,492 50,361 52,231 1,00 61,57	0
ATOM	1450	CB LEU A 497	42.210 52.946 50.981 1.00 58.80	С
		CG LEU A 497		С
ATOM		CD1 LEU A 497	40.717 54.877 51.444 1.00 65.00	С
ATOM		CD2 LEU A 497	42.982 54.819 52.483 1.00 64.40	С
ATOM	1454	N GLN A 498	42.840 50.016 50.116 1.00 57.38	N
ATOM		CA GLN A 498	42.669 48.597 50.349 1.00 55.74	С
	1456	C GLN A 498	44.011 47.986 50.680 1.00 55.51	С
ATOM		O GLN A 498	44.127 47.270 51.653 1.00 55.98	Ο
ATOM		CB GLN A 498	42.037 47.885 49.161 1.00 56.58	С
		CG GLN A 498	41.901 46.397 49.303 1.00 58.82	С
		CD GLN A 498	41.090 45.718 48.242 1.00 60.96	C
ATOM	1461	OE1 GLN A 498	41.304 45.928 47.056 1.00 63.68	0
ATOM	1462	NE2 GLN A 498	40.134 44.875 48.625 1.00 62.29	N
ATOM	1463	N GLN A 499	45.055 48.224 49.917 1.00 56.42	N
ATOM	1464	CA GLN A 499	46.365 47.642 50.216 1.00 56.77	С
ATOM	1465	C GLN A 499	46.910 48.083 51.571 1.00 54.48	C
ATOM	1466	O GLN A 499	47.614 47.301 52.223 1.00 52.93	O
ATOM	1467	CB GLN A 499	47.323 48.036 49.117 1.00 60.49	С
	1468	CG GLN A 499	46.899 47.577 47.720 1.00 63.18	C
		CD GLN A 499	47.943 48.181 46.768 1.00 66.27	С
		OE1 GLN A 499	48.011 49.401 46.687 1.00 64.80	Ο
		NE2 GLN A 499	48.689 47.282 46.139 1.00 67.90	N
		N GLN A 500	46.626 49.298 51.982 1.00 49.56	N
		CA GLN A 500	46.992 49.791 53.283 1.00 47.83	С
		C GLN A 500	46.508 48.888 54.400 1.00 48.48	С
		O GLN A 500	47.258 48.320 55.208 1.00 49.65	О
		CB GLN A 500	46.422 51.236 53.446 1.00 46.97	С
		CG GLN A 500	47.355 52.289 52.796 1.00 42.84	С
		CD GLN A 500	46.661 53.575 52.477 1.00 39.88	С
		OE1 GLN A 500	45.984 54.134 53.307 1.00 38.64	0
		<b>NE2 GLN A 500</b>		N
		N HIS A 501	45.190 48.672 54.480 1.00 47.29	N
		CA HIS A 501	44.552 47.861 55.505 1.00 42.58	С
		C HIS A 501	44.996 46.422 55.449 1.00 43.22	С

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	. 404	O THE A 501	45.204 45.723 56.460 1.00 45.13	Ο
ATOM		O HIS A 501 CB HIS A 501		C
ATOM			42.245 47.480 54.393 0.50 43.18	C
ATOM		CG AHIS A 501	42.483 49.360 55.390 0.50 43.53	Č
ATOM		CG BHIS A 501	41.395 48.280 53.648 0.50 44.55	N
ATOM	_	ND1AHIS A 501	42.849 50.353 56.286 0.50 45.90	N
ATOM		ND1BHIS A 501	42.849 30.333 30.280 0.50 43.30	C
ATOM		CD2AHIS A 501	41.577 49.916 54.558 0.50 42.37	Č
ATOM		CD2BHIS A 501	40.760 47.503 52.765 0.50 44.96	Č
ATOM	_	CEIAHIS A 501	42.205 51.471 55.986 0.50 46.12	C
ATOM		CE1BHIS A 501	41.192 46.251 52.879 0.50 41.39	N
ATOM		NE2AHIS A 501		N
ATOM		NE2BHIS A 501	41.427 51.225 54.935 0.50 44.23	N
ATOM		N GLN A 502	45.258 45.931 54.236 1.00 42.10	
ATOM		CA GLN A 502	45.665 44.544 54.122 1.00 40.55	C
ATOM		C GLN A 502	47.070 44.369 54.674 1.00 41.26	С
ATOM		O GLN A 502	47.223 43.325 55.308 1.00 39.67	0
ATOM		CB GLN A 502	45.696 44.016 52.715 1.00 41.12	C
ATOM		CG GLN A 502	44.574 44.566 51.860 1.00 40.32	C
ATOM		CD GLN A 502	44.320 43.508 50.808 1.00 42.78	C
ATOM		OE1 GLN A 502	43.242 42.927 50.851 1.00 49.36	0
ATOM		NE2 GLN A 502	45.312 43.328 49.986 1.00 41.14	N
<b>ATOM</b>		N ARG A 503	47.950 45.305 54.294 1.00 40.71	N
ATOM	1506	CA ARG A 503	49.327 45.244 54.774 1.00 37.17	C
<b>ATOM</b>	1507	C ARG A 503	49.317 45.458 56.299 1.00 35.75	C
<b>ATOM</b>	1508	O ARG A 503	49,915 44.683 57.058 1.00 33.57	0
<b>ATOM</b>	1509	CB ARG A 503	50.177 46.335 54.137 1.00 40.97	С
<b>ATOM</b>	1510	CG ARG A 503	51.671 46.162 54.431 1.00 45.67	С
ATOM	1511	CD ARG A 503	52.568 47.135 53.682 1.00 43.81	С
<b>ATOM</b>	1512	NE ARG A 503	53.964 46.879 53.959 1.00 40.13	N
<b>ATOM</b>	1513	CZ ARG A 503	54.707 45.888 53.566 1.00 40.13	С
<b>ATOM</b>	1514	NH1 ARG A 503	54.230 44.968 52.777 1.00 39.43	N
<b>ATOM</b>	1515	NH2 ARG A 503	55.981 45.772 53.975 1.00 41.35	N
<b>ATOM</b>	1516	N LEU A 504	48.556 46.448 56.780 1.00 33.53	N
<b>ATOM</b>	1517	CA LEU A 504	48.500 46.664 58.228 1.00 34.14	·C
<b>ATOM</b>	1518	C LEU A 504	48.137 45.336 58.897 1.00 35.62	С
<b>ATOM</b>	1519	O LEU A 504	48.825 44.902 59.816 1.00 38.42	0
<b>ATOM</b>	1520	CB LEU A 504	47.501 47.693 58.699 1.00 33.74	С
<b>ATOM</b>	1521	CG LEU A 504	47.267 47.904 60.186 1.00 32.73	С
<b>ATOM</b>	1522	CD1 LEU A 504	48.459 48.646 60.839 1.00 33.32	С
<b>ATOM</b>	1523	CD2 LEU A 504	46.035 48.786 60.445 1.00 28.14	С
ATOM	1524	N ALA A 505	47.091 44.663 58.408 1.00 34.89	N
		CA ALA A 505	46.765 43.384 59.027 1.00 30.63	С
		C ALA A 505	47.844 42.353 58.814 1.00 30.88	С
ATOM			48.122 41.505 59.677 1.00 29.79	Ο
		CB ALA A 505	45.417 42.908 58.511 1.00 32.54	С
		N GLN A 506	48.524 42.304 57.679 1.00 34.12	N
ATOM		CA GLN A 506	49.518 41.245 57.498 1.00 38.19	С
ATOM		C GLN A 506	50.601 41,441 58.544 1.00 36.89	С
ATOM		O GLN A 506	51.080 40.450 59.135 1.00 36.61	0

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		CB GLN A 506		C
ATOM		CG GLN A 506		C
ATOM		CD GLN A 506		C
<b>ATOM</b>		OE1 GLN A 506	50.344 41.868 53.225 1.00 58.50	0
ATOM	1537	NE2 GLN A 506	48.166 41.687 52.827 1.00 57.68	N
<b>ATOM</b>	1538	N LEU A 507	50.926 42.703 58.807 1.00 35.11	N
<b>ATOM</b>	1539	CA LEU A 507	51.952 42.976 59.826 1.00 32.90	С
<b>ATOM</b>	1540	C LEU A 507	51.478 42.609 61.209 1.00 32.31	С
ATOM	1541	O LEU A 507	52.136 41.729 61.799 1.00 32.90	Ο
ATOM	1542	CB LEU A 507	52.368 44.441 59.738 1.00 33.00	С
ATOM	1543	CG LEU A 507	53.124 44.781 58.436 1.00 30.90	С
<b>ATOM</b>	1544	CD1 LEU A 507	53.407 46.266 58.363 1.00 33.64	С
ATOM	1545	CD2 LEU A 507	54.326 43.898 58.353 1.00 26.56	С
ATOM	1546	N LEU A 508	50.381 43.190 61.720 1.00 29.06	N
ATOM	1547	CA LEU A 508	49.943 42.806 63.067 1.00 29.08	С
ATOM	1548	C LEU A 508	49.768 41.341 63.326 1.00 31.97	С
<b>ATOM</b>	1549	O LEU A 508	50.337 40.833 64.325 1.00 31.14	0
ATOM	1550	CB LEU A 508	48.726, 43.606 63.452 1.00 29.57	С
<b>ATOM</b>	1551	CG LEU A 508	48.966 45.119 63.181 1.00 30.98	С
ATOM	1552	CD1 LEU A 508	47.708 45.877 63.540 1.00 28.17	С
ATOM	1553	CD2 LEU A 508	50.185 45.594 63.945 1.00 25.29	С
ATOM	1554	N LEU A 509	49.333 40.542 62.333 1.00 31.90	N
ATOM	1555	CA LEU A 509	49.247 39.089 62.497 1.00 27.26	С
	1556	C LEU A 509	50.588 38.474 62.724 1.00 28.18	С
ATOM	1557	O LEU A 509	50.694 37.425 63.363 1.00 31.85	Ο
		CB LEU A 509	48.561 38.422 61.318 1.00 23.15	С
		CG LEU A 509	47.064 38.638 61.213 1.00 25.76	С
ATOM		CD1 LEU A 509	46.469 37.882 60.057 1.00 24.02	С
ATOM	1561	CD2 LEU A 509	46.383 38.201 62.553 1.00 22.70	С
ATOM		N ILE A 510	51.638 39.130 62.234 1.00 31.59	N
ATOM		CA ILE A 510	52.997 38.574 62.437 1.00 31.40	С
ATOM		C ILE A 510	53.334 38.772 63.913 1.00 30.63	С
ATOM	1565	O ILE A 510	54.010 37.877 64.420 1.00 31.28	Ο
ATOM		CB ILE A 510	54.010 39.169 61.483 1.00 34.47	С
		CG1 ILE A 510	53.979 38.367 60.163 1.00 37.44	C
		CG2 ILE A 510	55.464 39.221 61.979 1.00 36.20	С
		CD1 ILE A 510	54.284 39.292 58.957 1.00 38.44	С
		N LEUA511	52.783 39.785 64.592 1.00 27.44	N
		CA LEU A 511	53.047 39.907 66.021 1.00 28.51	С
		C LEU A 511	52.535 38.703 66.757 1.00 32.18	С
ATOM		O LEU A 511	53.240 38.241 67.686 1.00 38.66	Ο
ATOM		CB LEU A 511	52.586 41.207 66.631 1.00 27.31	С
		CG LEU A 511	53.002 42.452 65.796 1.00 28.29	С
		CD1 LEU A 511	52.496 43.707 66.420 1.00 24.10	С
		CD2 LEU A 511	54.528 42.469 65.580 1.00 24.27	C
ATOM			51.468 38.078 66.371 1.00 34.01	N
		CA SER A 512	50.960 36.841 66.927 1.00 34.05	С
ATOM			51.986 35.743 66.920 1.00 32.61	C
ATOM			52.133 35.062 67.931 1.00 36.28	0
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ATOM	1582 CB SER A 512	49.730 36.415 66.073 1.00 36.45	C
<b>ATOM</b>	1583 OG SER A 512	48.657 36.567 67.007 1.00 41.54	.0
ATOM	1584 N HIS A 513	52.716 35.584 65.839 1.00 32.89	N
<b>ATOM</b>	1585 CA HIS A 513	53.766 34.577 65.746 1.00 33.89	С
ATOM	1586 C HIS A 513	54.969 34.971 66.579 1.00 33.11	C
<b>ATOM</b>	1587 O HIS A 513	55.588 34.159 67.263 1.00 34.48	0
<b>ATOM</b>	1588 CB HIS A 513	54.201 34.456 64.285 1.00 37.72	C
ATOM	1589 CG HIS A 513	53.098 34.018 63.383 1.00 40.23	С
ATOM	1590 ND1 HIS A 513	52.317 32.930 63.699 1.00 45.67	N
ATOM	1591 CD2 HIS A 513	52.646 34.429 62.190 1.00 43.55	С
ATOM	1592 CE1 HIS A 513	51.403 32.727 62.765 1.00 44.13	С
ATOM	1593 NE2 HIS A 513	51.605 33.640 61.829 1.00 44.41	N
ATOM	1594 N ILE A 514	55.288 36.268 66.530 1.00 33.10	N
ATOM	1595 CA ILE A 514	56.433 36.756 67.334 1.00 31.94	С
ATOM	1596 C ILE A 514	56.104 36.408 68.766 1.00 32.61	С
ATOM	1597 O ILE A 514		0
ATOM	1598 CB ILE A 514	56.732 38.208 66.994 1.00 30.68	С
ATOM	1599 CG1 ILE A 514	57.427 38.276 65.644 1.00 32.27	С
ATOM	1600 CG2 ILE A 514	57.654 38.845 68.035 1.00 32.24	С
ATOM	1601 CD1 ILE A 514	57.666 39.646 65.073 1.00 31.53	С
ATOM	1602 N ARG A 515		N
ATOM	1603 CA ARG A 515	54.554 36.406 70.609 1.00 32.91	С
	1604 C ARG A 515		C
ATOM		55.158 34.423 71.871 1.00 30.76	0
ATOM	1606 CB ARG A 515	53.047 36.671 70.737 1.00 36.94	С
ATOM	1607 CG ARG A 515	52.620 36.398 72.202 1.00 34.83	С
ATOM	1608 CD ARG A 515	53.103 37.571 72.993 1.00 33.43	C
ATOM			N
ATOM	1610 CZ ARG A 515	51.518 39.040 74.027 1.00 40.22	С
ATOM	1611 NH1 ARG A 515	5 51.830 39.947 73.130 1.00 44.71	N
ATOM	1612 NH2 ARG A 51:	5 50.638 39.215 74.964 1.00 46.87	Ņ
ATOM	1613 N HIS A 516	54.238 34.150 69.837 1.00 36.19	N
ATOM		54.282 32.686 69.913 1.00 36.21	С
	1615 C HIS A 516	55.707 32.263 70.118 1.00 35.50	С
ATOM	1616 O HIS A 516	55.992 31.511 71.047 1.00 38.53	0
ATOM	1617 CB HIS A 516	53.671 32.077 68.655 1.00 39.92	С
ATOM	1618 CG HIS A 516	53.546 30.583 68.789 1.00 43.85	С
ATOM	1619 ND1 HIS A 516		N
ATOM	1620 CD2 HIS A 516	54.254 29.565 68.272 1.00 43.36	С
ATOM	1621 CE1 HIS A 516	52.671 28.702 69.525 1.00 42.83	С
ATOM	1622 NE2 HIS A 516	53.682 28.417 68.754 1.00 44.73	N
ATOM		56.642 32.758 69.280 1.00 34.02	N
ATOM	1624 CA MET A 517	58.044 32.363 69.496 1.00 33.79	С
ATOM	1625 C MET A 517	58.582 32.756 70.860 1.00 33.49	С
ATOM		59.128 31.928 71.588 1.00 35.14	0
ATOM		58.907 32.894 68.379 1.00 33.68	C
ATOM		58.635 32.256 67.047 1.00 34.56	С
ATOM		59.379 33.052 65.684 1.00 39.78	S
	1630 CE MET A 517	58.650 34.676 65.728 1.00 36.45	С

	1621 N. OED A 610	50 207 22 222 71 201 1 20 22 17	N.T
		58.287 33.932 71.391 1.00 32.17	N
		58.814 34.255 72.728 1.00 33.21	C
ATOM	1633 C SER A 518	58.258 33.351 73.810 1.00 34.37	C
ATOM	1634 O SER A 518	59.026 32.919 74.699 1.00 30.18	0
ATOM		58.660 35.740 73.023 1.00 31.26	C
ATOM	1636 OG SER A 518	58.344 35.917 74.367 1.00 28.79	0
ATOM	1637 N ASN A 519	56.954 33.031 73.778 1.00 32.58	N
ATOM	1638 CA ASN A 519	56.470 32.071 74.778 1.00 33.07	С
ATOM		57.147 30.732 74.586 1.00 37.75	С
ATOM		57.570 30.029 75.506 1.00 35.09	0
ATOM		54.992 31.804 74.532 1.00 34.03	С
ATOM	1642 CG ASN A 519	54.162 33.022 74.946 1.00 32.85	С
<b>ATOM</b>	1643 OD1 ASN A 519	54.541 33.610 75.938 1.00 29.80	O
<b>ATOM</b>	1644 ND2 ASN A 519	53.088 33.307 74.226 1.00 33.79	N
<b>ATOM</b>	1645 N LYS A 520	57.315 30.322 73.285 1.00 41.23	N
<b>ATOM</b>	1646 CA LYS A 520	57.986 28.990 73.213 1.00 44.55	С
ATOM	1647 C LYS A 520	59.387 29.139 73.775 1.00 46.06	С
ATOM	1648 O LYS A 520	59.917 28.260 74.463 1.00 49.52	0
ATOM	1649 CB LYS A 520	57.968 28.446 71.812 1.00 47.67	С
ATOM	1650 CG LYS A 520	56.670 27.855 71.277 1.00 49.96	С
ATOM	1651 CD LYS A 520		С
ATOM	1652 CE LYS A 520		С
ATOM	1653 NZ LYS A 520	55.534 25.198 73.469 1.00 59.42	N
ATOM	1654 N GLY A 521	60.058 30.267 73.515 1.00 41.38	N
ATOM	1655 CA GLY A 521	61.432 30.412 73.867 1.00 39.78	C
ATOM	1656 C GLY A 521	61.658 30.534 75.347 1.00 40.02	C
ATOM	1657 O GLY A 521	62.701 30.165 75.890 1.00 41.28	Ō
ATOM	1658 N MET A 522	60.678 31.118 75.998 1.00 41.42	N
ATOM	1659 CA MET A 522	60.768 31.349 77.433 1.00 42.08	C
ATOM	1660 C MET A 522	60.717 30.041 78.162 1.00 49.07	C
ATOM	1661 O MET A 522	61,509 29.838 79.085 1.00 56.07	ŏ
ATOM	1662 CB MET A 522	59.684 32.291 77.829 1.00 39.53	C
ATOM	1663 CG MET A 522	60.157 33.731 77.541 1.00 42.45	Č
	1664 SD MET A 522	59.509 34.694 78.912 1.00 49.75	S
	1665 CE MET A 522	58.965 36.121 77.995 1.00 43.03	C
	1666 N GLU A 523	59.893 29.147 77.687 1.00 43.03	N
	1667 CA GLU A 523	59.767 27.782 78.081 1.00 58.80	C
			c
	1668 C GLU A 523	61.095 27.061 77.843 1.00 60.25	
	1669 O GLU A 523	61.546 26.303 78.661 1.00 61.66	0
	1670 CB GLU A 523	58.760 27.032 77.156 1.00 60.53	C
	1671 CG GLU A 523	57.490 26.591 77.833 1.00 65.10	C
	1672 CD GLU A 523		C
	1673 OE1 GLU A 523	56.619 24.909 76.435 1.00 72.53	C
	1674 OE2 GLU A 523	55.526 26.874 76.438 1.00 69.51	C
ATOM		61.659 27.262 76.658 1.00 64.23	N
	1676 CA HIS A 524	62.914 26.551 76.369 1.00 68.36	C
	1677 C HIS A 524	64.007 27.149 77.237 1.00 68.67	C
	1678 O HIS A 524	64.733 26.419 77.903 1.00 66.17	0
ATOM	1679 CB HIS A 524	63.178 26.544 74.894 1.00 71.77	С

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ATOM	1680 CG HIS A 524	64.579 26.275 74.474 1.00 76.25	С
ATOM		65.129 26.831 73.329 1.00 77.80	N
ATOM	1682 CD2 HIS A 524	65.544 25.505 75.037 1.00 78.01	С
ATOM	1683 CE1 HIS A 524	66.375 26.406 73.210 1.00 79.59	С
ATOM	1684 NE2 HIS A 524	66.650 25.604 74.228 1.00 80.79	N
ATOM	1685 N LEU A 525	64.000 28.462 77.419 1.00 69.72	N
ATOM	1686 CA LEU A 525	64,976 29.072 78.309 1.00 73.19	C
ATOM	1687 C LEU A 525	64.853 28.613 79.748 1.00 78.52	C
ATOM		65.872 28.438 80.422 1.00 78.86	0
ATOM	1689 CB LEU A 525	64.874 30.586 78.208 1.00 69.41	С
<b>ATOM</b>	1690 CG LEU A 525	66.064 31.385 77.682 1.00 65.43	C
<b>ATOM</b>	1691 CD1 LEU A 525	66.814 30.680 76.575 1.00 62.25	С
<b>ATOM</b>	1692 CD2 LEU A 525	65.590 32.752 77.232 1.00 63.11	С
ATOM	1693 N TYR A 526	63.651 28.440 80.291 1.00 85.31	N
<b>ATOM</b>	1694 CA TYR A 526	63.483 28.045 81.682 1.00 90.81	С
<b>ATOM</b>	1695 C TYR A 526	63.638 26.558 81.891 1.00 91.90	C
<b>ATOM</b>		64.032 26.161 82.998 1.00 92.38	Ο
<b>ATOM</b>	1697 CB TYR A 526	62.194 28.564 82.270 1.00 97.06	С
<b>ATOM</b>		62.120 30.071 82.388 1.00104.66	С
<b>ATOM</b>		63.144 30.909 81.961 1.00106.68	C
<b>ATOM</b>	1700 CD2 TYR A 526	60.990 30.678 82.945 1.00107.36	C
<b>ATOM</b>		63.055 32.271 82.078 1.00108.14	С
ATOM		60.893 32.052 83.067 1.00109.12	·C
ATOM		61.937 32.845 82.629 1.00109.89	С
<b>ATOM</b>		61.841 34.218 82.752 1.00111.92	0
<b>ATOM</b>	1705 N SER A 527		N
ATOM	1706 CA SER A 527	63.790 24.328 80.992 1.00 95.45	С
ATOM	1707 C SER A 527	65.289 24.118 81.235 1.00 99.20	C
ATOM			0
	1709 CB SER A 527		C
		63.891 23.821 78.591 1.00 90.22	0
		66.130 24.898 80.579 1.00102.07	N
		67.568 24.846 80.673 1.00102.85	C
	1713 C MET A 528	68.047 25.302 82.050 1.00105.63	C
	1714 O MET A 528	68.088 24.486 82.976 1.00108.44	0
	1715 CB MET A 528	68.203 25.715 79.584 1.00100.04	C
	1716 CG MET A 528	68.106 25.183 78.174 1.00 97.06	C
	1717 SD MET A 528	68.537 26.345 76.869 1.00 93.64	S C
	1718 CE MET A 528	69.354 27.655 77.751 1.00 94.41	
	1719 N PRO A 535	63.567 37.472 88.984 1.00 87.02	N C
	1720 CA PRO A 535	64.688 38.390 89.191 1.00 83.59	
	1721 C PRO A 535	64.668 39.490 88.133 1.00 77.41	C O
ATOM		64.982 40.657 88.436 1.00 76.08	C
ATOM		65.996 37.567 89.158 1.00 85.89	C
ATOM		65.508 36.152 89.030 1.00 87.24	C
	1725 CD PRO A 535	64.069 36.136 88.567 1.00 87.96	N
	1726 N LEU A 536	64.112 39.148 86.959 1.00 68.79	C
ATOM		64.158 40.084 85.833 1.00 61.48	C
ATOM	1728 C LEU A 536	63.555 41.427 86.201 1.00 56.92	C

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ATOM		O LEU A 536		0
<b>ATOM</b>	1730	CB LEU A 536	63.499 39.485 84.625 1.00 61.82	С
<b>ATOM</b>	1731	CG LEU A 536	63.456 40.289 83.359 1.00 61.94	С
ATOM	1732	CD1 LEU A 536	64.733 41.039 83.096 1.00 66.59	С
<b>ATOM</b>	1733	CD2 LEU A 536	63.167 39.343 82.203 1.00 65.06	С
<b>ATOM</b>	1734	N TYR A 537	62.461 41.317 86.973 1.00 52.04	N
<b>ATOM</b>	1735	CA TYR A 537	61.734 42.468 87.440 1.00 49.60	С
ATOM	1736	C TYR A 537	62.672 43.440 88.136 1.00 52.75	С
ATOM	1737	O TYR A 537	62.753 44.649 87.884 1.00 46.82	0
<b>ATOM</b>	1738	CB TYR A 537	60.631 42.061 88.410 1.00 46.96	С
ATOM	1739	CG TYR A 537	59.869 43.265 88.887 1.00 48.55	С
ATOM	1740	CD1 TYR A 537	60.333 44.054 89.909 1.00 51.84	С
ATOM	1741	CD2 TYR A 537	58.668 43.647 88.318 1.00 53.37	С
ATOM	1742	CE1 TYR A 537	59.665 45.180 90.357 1.00 54.70	С
ATOM	1743	CE2 TYR A 537	57.946 44.761 88.732 1.00 54.40	С
ATOM	1744	CZ TYR A 537	58.468 45.525 89.751 1.00 57.28	С
ATOM	1745	OH TYR A 537	57.796 46.659 90.174 1.00 60.33	0
ATOM	1746	N ASP A 538	63.393 42.826 89.102 1.00 58.32	N
ATOM	1747	CA ASP A 538	64.281 43.628 89.951 1.00 62.64	C
<b>ATOM</b>	1748	C ASP A 538	65.375 44.203 89.079 1.00 61.73	С
<b>ATOM</b>	1749	O ASP A 538	65.730 45.378 89.192 1.00 64.00	Ο
<b>ATOM</b>	1750	CB ASP A 538	64.775 42.811 91.106 1.00 70.68	С
<b>ATOM</b>	1751	CG ASP A 538	63.674 42.219 91.974 1.00 75.57	C
<b>ATOM</b>	1752	OD1 ASP A 538	62.509 42.664 91.885 1.00 75.31	Ο
ATOM	1753	OD2 ASP A 538	64.007 41.294 92.777 1.00 78.95	0
<b>ATOM</b>	1754	N LEU A 539	65.864 43.356 88.177 1.00 58.42	N
<b>ATOM</b>	1755	CA LEU A 539	66.891 43.778 87.247 1.00 56.11	С
<b>ATOM</b>	1756	C LEU A 539	66.464 44.977 86.424 1.00 55.33	С
<b>ATOM</b>	1757	O LEU A 539	67.198 45.960 86.300 1.00 56.67	Ο
<b>ATOM</b>	1758	CB LEU A 539	67.152 42.613 86.314 1.00 59.46	С
<b>ATOM</b>	1759	CG LEU A 539	68.591 42.098 86.337 1.00 63.12	С
<b>ATOM</b>	1760	CD1 LEU A 539	68.627 40.824 85.472 1.00 66.12	С
<b>ATOM</b>	1761	CD2 LEU A 539	69.575 43.132 85.869 1.00 63.42	С
<b>ATOM</b>	1762	N LEU A 540	65.286 44.888 85.814 1.00 52.86	N
<b>ATOM</b>	1763	CA LEU A 540	64.782 45.949 84.965 1.00 50.07	С
<b>ATOM</b>	1764	C LEU A 540	64.505 47.193 85.780 1.00 50.03	С
<b>ATOM</b>	1765	O LEU A 540	64.704 48.340 85.350 1.00 45.66	Ο
<b>ATOM</b>	1766	CB LEU A 540	63.513 45.418 84.280 1.00 51.61	С
<b>ATOM</b>	1767	CG LEU A 540	63.707 44.278 83.279 1.00 50.39	С
<b>ATOM</b>	1768	CD1 LEU A 540	62.415 43.605 82.952 1.00 47.32	С
<b>ATOM</b>	1769	CD2 LEU A 540	64.353 44.785 81.982 1.00 52.21	С
<b>ATOM</b>	1770	N LEU A 541	64.026 46.945 87.007 1.00 52.25	N
<b>ATOM</b>	1771	CA LEU A 541	63.724 48.073 87.898 1.00 56.18	С
<b>ATOM</b>	1772	C LEU A 541	65.035 48.788 88.182 1.00 57.88	С
<b>ATOM</b>	1773	O LEU A 541	65.174 50.004 88.001 1.00 58.33	Ο
<b>ATOM</b>	1774	CB LEU A 541	63.083 47.605 89.201 1.00 59.40	С
<b>ATOM</b>	1775	CG LEU A 541	62.606 48.642 90.209 1.00 59.00	С
<b>ATOM</b>	1776	CD1 LEU A 541	62.558 50.048 89.660 1.00 60.26	С
ATOM	1777	CD2 LEU A 541	61.208 48.296 90.704 1.00 58.85	С

ATOM	1778	N GLU A 542	66.025 47.944 88.573 1.00 56.65	N
			67.343 48.545 88.816 1.00 57.17	С
			67.772 49.230 87.534 1.00 58.47	С
ATOM	1781			0
ATOM			68.331 47.543 89.336 1.00 56.35	С
ATOM			67.805 48.491 86.424 1.00 57.50	N
			68.200 49.160 85.176 1.00 60.04	C
		C MET A 543	_	C
	1790		67.911 51.423 84.433 1.00 51.56	Ö
			68.226 48.108 84.077 1.00 62.92	C
			69.541 47.326 84.027 1.00 65.16	Č
			69.416 46.065 82.729 1.00 65.51	S
			68.490 44.802 83.540 1.00 63.57	C
ATOM			66.019 50.253 84.860 1.00 61.14	N
ATOM			65.209 51.402 84.496 1.00 62.86	Č
				C
			65.454 52.572 85.437 1.00 68.07	
			65.323 53.711 84.983 1.00 66.46	0
			63.749 51.090 84.425 1.00 61.05	C
			63.154 50.387 83.217 1.00 58.33	C
			61.836 49.732 83.583 1.00 54.05	C
ATOM			62.994 51.351 82.067 1.00 58.50	С
ATOM			65.666 52.308 86.735 1.00 75.95	N
			65.833 53.447 87.631 1.00 84.89	C.
		C ASP A 545		C
ATOM			67.231 55.336 87.351 1.00 88.95	0
			65.567 53.176 89.095 1.00 89.55	С
			64.831 54.302 89.816 1.00 <b>92.87</b>	С
<b>ATOM</b>	1809	OD1 ASP A 545	64.559 55.367 89.211 1.00 93.84	0
<b>ATOM</b>	1810	OD2 ASP A 545	64.502 54.146 91.022 1.00 94.22	0
<b>ATOM</b>	1811	N ALA A 546	68.241 53.319 87.265 1.00 91.11	N
<b>ATOM</b>	1812	CA ALA A 546	69.593 53.826 87.034 1.00 94.05	С
ATOM	1813	C ALA A 546	69.635 54.811 85.873 1.00 95.87	С
			70.073 55.952 86.001 1.00 97.17	Ο
		CB ALA A 546		C ·
		N HIS A 547	69.124 54.397 84.727 1.00 97.69	N
			68.937 55.242 83.573 1.00 99.06	C
		C HIS A 547	68.772 56.714 83.958 1.00 98.07	С
		O HIS A 547	69.164 57.583 83.141 1.00 95.96	0
			67.659 54.755 82.832 1.00100.43	C
			67.688 55.178 81.391 1.00101.48	С
		ND1 HIS A 547		N
		CD2 HIS A 547	68.612 54.876 80.435 1.00101.27	C
		CE1 HIS A 547		Č
		NE2 HIS A 547		N
TER 1		HIS A 547	08.224 55.515 75.255 1.00100.01	• `
		. HIS A 347 27 C1 ACBM A 38	54.836 38.076 80.880 0.50 61.38	С
				c
		28 C1 BCBM A 38		C
		9 C2 ACBM A 38		C
HETAT	M 183	0 C2 BCBM A 38	54.097 38.891 79.955 0.50 57.13	C

		55.146 37.147 79.993 0.50 61.86	0
	O1 BCBM A 381		0
	O2 ACBM A 381		0
	O2 BCBM A 381		0
HETATM 1835	C1 RAL A 600	69.571 36.223 71.917 1.00 31.33	С
	C2 RAL A 600	69.816 37.448 71.352 1.00 30.47	С
HETATM 1837	C3 RAL A 600	69.083 37.933 70.305 1.00 31.66	С
HETATM 1838	O3 RAL A 600	69.410 39.186 69.850 1.00 32.81	0
<b>HETATM</b> 1839	C4 RAL A 600	68.029 37.167 69.794 1.00 33.99	С
HETATM 1840	C5 RAL A 600	67.765 35.956 70.385 1.00 33.49	С
HETATM 1841	S6 RAL A 600	66.638 34.815 69.986 1.00 33.96	S
<b>HETATM 1842</b>	C7 RAL A 600	67.001 33.691 71.192 1.00 34.48	С
<b>HETATM 1843</b>	C8 RAL A 600	66.347 32.356 71.301 1.00 35.62	С
HETATM 1844	C9 RAL A 600	66.087 31.727 70.099 1.00 35.20	С
HETATM 1845	C10 RAL A 600	65.560 30.446 70.128 1.00 38.32	С
<b>HETATM 1846</b>	C11 RAL A 600	65.259 29.817 71.320 1.00 39.44	С
<b>HETATM 1847</b>	O11 RAL A 600	64.735 28.525 71.249 1.00 46.17	Ο
<b>HETATM 1848</b>	C12 RAL A 600	65.562 30.428 72.519 1.00 36.17	С
<b>HETATM</b> 1849	C13 RAL A 600	66.106 31.706 72.480 1.00 34.51	С
HETATM 1850	C14 RAL A 600	68.556 35.468 71.464 1.00 31.87	С
HETATM 1851	C15 RAL A 600	68.128 34.150 71.906 1.00 33.10	С
<b>HETATM 1852</b>	C16 RAL A 600	68.771 33.463 72.918 1.00 36.94	С
HETATM 1853	O16 RAL A 600	69.368 32.412 72.653 1.00 40.67	Ο
HETATM 1854	C17 RAL A 600	68,768 33.917 74.313 1.00 36.96	С
HETATM 1855	C18 RAL A 600	69.621 33.351 75.239 1.00 34.73	С
HETATM 1856	C19 RAL A 600	69.633 33.745 76.563 1.00 34.67	С
HETATM 1857	C20 RAL A 600	68,733 34,725 76.978 1.00 37.20	С
HETATM 1858	C21 RAL A 600	67.879 35.305 76.057 1.00 40.93	С
<b>HETATM 1859</b>	C22 RAL A 600	67.907 34.910 74.730 1.00 39.84	С
<b>HETATM 1860</b>	O23 RAL A 600	68.555 35.259 78.220 1.00 36.45	Ο
HETATM 1861	C24 RAL A 600	69.461 34.837 79.228 1.00 38.03	С
<b>HETATM 1862</b>	C25 RAL A 600	69.311 35.692 80.458 1.00 43.08	С
<b>HETATM 1863</b>	N26 RAL A 600	69.023 37.110 80.557 1.00 46.61	N
HETATM 1864	C27 RAL A 600	68.720 37.437 81.965 1.00 47.65	С
HETATM 1865	C28 RAL A 600	68.544 38.946 82.229 1.00 48.95	С
HETATM 1866	C29 RAL A 600	67.338 39.404 81.393 1.00 50.06	С
HETATM 1867	C30 RAL A 600	67.804 39.197 79.919 1.00 50.91	С
HETATM 1868	C31 RAL A 600	67.960 37.681 79.707 1.00 50.67	С
ATOM 1869 N	1 LEU B 306	36.674 30.066 44.727 1.00 91.06	N
ATOM 1870 C	CA LEUB 306	35.325 30.211 45.360 1.00 93.16	С
ATOM 1871 C	C LEU B 306	35.377 31.143 46.562 1.00 89.78	С
ATOM 1872 (	LEU B 306	34.800 32.241 46.512 1.00 87.52	0
ATOM 1873 C	CB LEUB 306	34.709 28.870 45.748 1.00 97.18	С
ATOM 1874 (	CG LEUB 306	33.305 28.821 46.303 1.00101.83	С
ATOM 1875 C		32.367 29.926 45.882 1.00102.32	С
ATOM 1876 C		32.733 27.433 46.075 1.00103.20	С
ATOM 1877 N	N ALA B 307	36.135 30.778 47.577 1.00 87.24	N
ATOM 1878 (	CA ALAB 307	36.337 31.584 48.780 1.00 84.71	С
ATOM 1879 (	C ALA B 307	36.798 33.005 48.496 1.00 81.15	С

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ATOM	1880	O ALA B 307	36.351 33.998 49.052 1.00 79.11	O
			37.375 30.869 49.647 1.00 84.65	C
		N LEUB 308		N
		CA LEU B 308	38.271 34.398 47.137 1.00 79.21	C
		C LEU B 308	37.313 35.245 46.327 1.00 76.88	C
ATOM		O LEU B 308		ŏ
		CB LEU B 308		Č
		CG LEU B 308		Č
		CD1 LEU B 308	41.773 33.104 46.143 1.00 80.23	C
		CD2 LEU B 308	41.238 34.558 48.122 1.00 78.18	č
		N SER B 309	36.187 34.682 45.937 1.00 74.71	N
		CA SER B 309	35.273 35.475 45.127 1.00 74.21	C
		C SER B 309	34.123 36.021 45.944 1.00 71.62	c
_		O SER B 309		Ö
		CB SER B 309		C
ATOM			34.808 33.289 44.133 1.00 76.34	Ö
		N LEUB 310	34.013 35.699 47.224 1.00 66.47	N
		CA LEUB 310	32.894 36.171 48.028 1.00 62.19	C
		C LEUB 310		C
ATOM		O LEUB 310		0
			32.908 35.534 49.430 1.00 60.65	C
ATOM		CG LEU B 310		C
ATOM			32.907 33.539 50.906 1.00 61.50	С
ATOM		CD2 LEU B 310	31.497 33.570 48.834 1.00 57.77	С
ATOM		N THR B 311	31.763 38.276 48.470 1.00 57.68	N
ATOM	1905	CA THR B 311	31.802 39.704 48.787 1.00 56.79	С
ATOM	1906	C THR B 311	32.008 39.830 50.298 1.00 55.01	С
ATOM	1907	O THR B 311	32.030 38.818 50.985 1.00 52.51	Ο
<b>ATOM</b>	1908	CB THR B 311	30.554 40.446 48.308 1.00 55.64	C
ATOM	1909	OG1 THR B 311	29.386 39.919 48.896 1.00 54.85	• 0
<b>ATOM</b>	1910	CG2 THR B 311	30.473 40.352 46.792 1.00 54.89	С
ATOM	1911	N ALA B 312	32.152 41.040 50.812 1.00 53.60	N
			32.287 41.245 52.256 1.00 49.90	C
			31.033 40.697 52.891 1.00 49.90	C ·
			31.143 39.803 53.723 1.00 51.10	0
ATOM	1915	CB ALA B 312	32.495 42.684 52.645 1.00 45.67	С
		N ASP B 313	29.852 41.129 52.428 1.00 52.72	N
		CA ASP B 313	28.645 40.569 53.019 1.00 56.00	С
		C ASP B 313	28.443 39.070 52.837 1.00 54.55	C
		O ASP B 313		0
			27.355 41.243 52.657 1.00 56.17	C
			27.253 42.696 52.951 1.00 58.96	C
		ODI ASP B 313	27.527 43.200 54.061 1.00 58.70	0
ATOM			26.891 43.365 51.949 1.00 62.08	0
		N GLN B 314	28.978 38.417 51.824 1.00 54.51	N
		CA GLN B 314	28.733 36.979 51.697 1.00 56.64	C
		C GLN B 314	29.567 36.196 52.694 1.00 55.43	С
			29.141 35.222 53.305 1.00 57.31	0
ATOM	1928	CB GLN B 314	29.002 36.513 50.279 1.00 57.95	С

28.127 37.253 49.263 1.00 57.78 C ATOM 1929 CG GLN B 314 ATOM 1930 CD GLN B 314 28.553 36.909 47.852 1.00 58.32 29,718 36,910 47,470 1.00 57.50 0 ATOM 1931 OE1 GLN B 314 N 27.523 36.594 47.098 1.00 60.62 ATOM 1932 NE2 GLN B 314 ATOM 1933 N MET B 315 30.754 36.685 52.891 1.00 52.23 N C ATOM 1934 CA MET B 315 31.739 36.241 53.827 1.00 49.70 ATOM 1935 C MET B 315 31.133 36.254 55.234 1.00 46.39 C 31.194 35.291 55.998 1.00 41.29 ATOM 1936 O MET B 315 0 ATOM 1937 CB MET B 315 32.848 37.320 53.756 1.00 52.35 33.985 37.099 54.749 1.00 54.04 ATOM 1938 CG MET B 315 35.044 35.772 54.203 1.00 56.39 ATOM 1939 SD MET B 315 ATOM 1940 CE MET B 315 34.543 34.408 55.191 1.00 56.31 ATOM 1941 N VAL B 316 30.591 37.428 55.579 1.00 42.31 N C ATOM 1942 CA VAL B 316 29.993 37.536 56.893 1.00 42.79 ATOM 1943 C VAL B 316 28.882 36.517 57.087 1.00 41.54 C ATOM 1944 O VAL B 316 28.898 35.860 58.125 1.00 43.23 0 29.401 38.908 57.216 1.00 41.66 C ATOM 1945 CB VAL B 316 28.789 38.844 58.592 1.00 41.71 C ATOM 1946 CG1 VAL B 316 ATOM 1947 CG2 VAL B 316 30.437 39.993 57.108 1.00 44.09 C 27.937 36.398 56.163 1.00 40.87 ATOM 1948 N SER B 317 N C ATOM 1949 CA SER B 317 26.845 35.448 56.455 1.00 44.95 ATOM 1950 C SER B 317 27.340 34.030 56.379 1.00 42.50 C 26.880 33.149 57.086 1.00 42.42 ATOM 1951 O SER B 317 0 C 25.636 35.630 55.554 1.00 46.95 ATOM 1952 CB SER B 317 26.099 35.778 54.245 1.00 51.75 0 ATOM 1953 OG SER B 317 28.324 33.767 55.504 1.00 40.11 ATOM 1954 N ALA B 318 N ATOM 1955 CA ALA B 318 28.795 32.377 55.488 1.00 38.46 C 29.217 32.030 56.928 1.00 40.51 C ATOM 1956 C ALA B 318 28.959 30.989 57.494 1.00 42.17 0 ATOM 1957 O ALA B 318 C ATOM 1958 CB ALA B 318 29,920 32,190 54,554 1.00 32,54 29.968 32.952 57.500 1.00 42.20 N ATOM 1959 N LEUB 319 C ATOM 1960 CA LEU B 319 30.565 32.839 58.786 1.00 39.71 ATOM 1961 C LEUB 319 29.546 32.729 59.904 1.00 40.27 C 29.688 31.814 60.716 1.00 37.79 ATOM 1962 O LEUB 319 0 C 31.495 34.038 58.998 1.00 33.71 ATOM 1963 CB LEUB 319 ATOM 1964 CG LEU B 319 32.768 33.858 58.194 1.00 31.85 ATOM 1965 CD1 LEU B 319 33.727 35.029 58.472 1.00 33.62 33.378 32.498 58.401 1.00 26.82 C ATOM 1966 CD2 LEU B 319 ATOM 1967 N LEUB 320 28.591 33.630 59.877 1.00 41.15 N 27.523 33.694 60.871 1.00 41.53 C ATOM 1968 CA LEU B 320 ATOM 1969 C LEUB 320 26.745 32.394 60.833 1.00 45.93 C 26.314 31.873 61.869 1.00 49.20 ATOM 1970 O LEUB 320 0 C ATOM 1971 CB LEUB 320 26.591 34.866 60.594 1.00 36.95 27.082 36.214 61.131 1.00 37.97 ATOM 1972 CG LEU B 320 ATOM 1973 CD1 LEU B 320 26.133 37.337 60.825 1.00 33.54 C C ATOM 1974 CD2 LEU B 320 27.335 36.118 62.636 1.00 35.35 ATOM 1975 N ASP B 321 26.663 31.823 59.644 1.00 47.02 N ATOM 1976 CA ASP B 321 26.010 30.577 59.440 1.00 50.66 C ATOM 1977 C ASP B 321 26.740 29.406 60.030 1.00 46.60 C

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		O ASP B 321		0
ATOM			25.910 30.237 57.913 1.00 59.17	C
ATOM			24.471 29.735 57.741 1.00 63.60	C
ATOM			23.615 30.631 57.906 1.00 64.90	0
ATOM			24.323 28.523 57.513 1.00 66.90	0
ATOM		N ALAB 322		N
ATOM		CA ALAB 322		C
ATOM		C ALA B 322		C
ATOM		O ALAB 322		0
ATOM		CB ALAB 322	30.218 28.587 59.801 1.00 32.90	C
ATOM		N GLUB 323		N
ATOM			28.626 29.441 64.129 1.00 35.05	С
ATOM		C GLU B 323		C
ATOM		O GLU B 323		0
ATOM		CB GLUB 323		C
ATOM			28.693 31.894 64.759 1.00 35.65	C
ATOM			29,907 31.568 65.638 1.00 37.28	C
ATOM			30.881 31.084 65.044 1.00 37.53	0
ATOM		OE2 GLU B 323		.0
ATOM			29.069 27.613 65.654 1.00 37.32	N
		CA PRO B 324		C
		C PRO B 324		C
ATOM			27.445 27.974 67.725 1.00 35.69	0
ATOM			29.926 25.912 67.120 1.00 36.62	C
ATOM			30.795 27.125 67.154 1.00 35.28	C
ATOM			30.285 28.185 66.199 1.00 37.93	C
ATOM		N PRO B 325		N
ATOM		CA PROB 325		С
ATOM		C PRO B 325		C
ATOM		O PRO B 325		0
ATOM		CB PRO B 325		C
ATOM			26.275 23.689 68.477 1.00 30.29	C
ATOM			27.141 24.441 67.507 1.00 32.36	C
ATOM		N ILE B 326	25.929 27.031 71.231 1.00 35.84	N
		CA ILE B 326	26.567 27.139 72.555 1.00 36.70	С
		C ILE B 326	26.240 25.913 73.382 1.00 38.88	С
ATOM			25.058 25.724 73.698 1.00 42.79	0
		CB ILE B 326	26.123 28.433 73.253 1.00 37.21	С
		CG1 ILE B 326	26.777 29.593 72.434 1.00 35.81	C
		CG2 ILE B 326	26.616 28.473 74.693 1.00 32.67	C
		CD1 ILE B 326	26.211 30.920 72.862 1.00 41.70	С
		N LEU B 327	27.179 25.020 73.679 1.00 35.51	N
		CA LEUB 327	26.891 23.820 74.412 1.00 30.60	С
		C LEU B 327	26.734 24.065 75.899 1.00 35.93	C
		O LEU B 327	27.083 25.118 76.388 1.00 38.14	0
		CB LEUB 327	28.035 22.821 74.220 1.00 30.41	C
		CG LEUB 327		C
		CD1 LEU B 327		C
ATOM	2026	CD2 LEU B 327	27.149 22.038 71.986 1.00 33.00	С

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ATOM	2027	N TYR B 328	26.248 23.082 76.662 1.00 38.95	N
ATOM	2028	CA TYR B 328	26.048 23.110 78.065 1.00 39.09	С
ATOM	2029	C TYR B 328	26.937 22.118 78.795 1.00 40.90	С
ATOM	2030	O TYR B 328	27.340 21.115 78.209 1.00 37.06	O
ATOM	2031	CB TYR B 328	24.637 22.721 78.470 1.00 43.01	С
ATOM	2032	CG TYR B 328	23.637 23.835 78.325 1.00 45.81	С
ATOM		CD1 TYR B 328	23.193 24.252 77.073 1.00 43.80	С
ATOM		CD2 TYR B 328	23.148 24.465 79.472 1.00 46.54	С
ATOM		CE1 TYR B 328	22.264 25.251 76.964 1.00 44.96	С
ATOM		CE2 TYR B 328	22,222 25,499 79,356 1.00 45.50	С
ATOM		CZ TYR B 328	21.799 25.880 78.103 1.00 46.55	С
ATOM		OH TYR B 328	20.868 26.894 77.991 1.00 48.51	0
ATOM	2039		27.188 22.518 80.048 1.00 45.16	N
ATOM		CA SER B 329	28.030 21.679 80.884 1.00 50.48	С
ATOM	2041		27.211 20.428 81.217 1.00 53.86	С
ATOM	2042		26.079 20.598 81.626 1.00 55.54	0
ATOM		CB SER B 329	28.437 22.309 82.217 1.00 47.00	С
ATOM		OG SER B 329	29.422 21.345 82.720 1.00 47.21	Ο
ATOM	2045		27.732 19.283 81.042 1.00 59.98	N
ATOM		CA GLUB 330	26.998 18.042 81.324 1.00 70.19	С
ATOM		C GLU B 330	27.154 17.795 82.810 1.00 76.09	С
ATOM			28.098 17.104 83.179 1.00 78.83	0
ATOM		CB GLUB 330	27.633 16.977 80.487 1.00 72.08	С
ATOM		CG GLUB 330	26.915 15.690 80.194 1.00 74.06	С
ATOM		CD GLU B 330	27.861 14.891 79.282 1.00 76.03	С
ATOM		OE1 GLU B 330	28.322 15.500 78.291 1.00 77.49	0
ATOM		<b>OE2 GLU B 330</b>	28.109 13.726 79.613 1.00 76.55	0
ATOM	2054		26.292 18.399 83.607 1.00 83.66	N
ATOM		CA TYR B 331	26.452 18.272 85.060 1.00 91.44	С
ATOM	2056	C TYR B 331	25,131 18.314 85.781 1.00 92.28	С
ATOM	2057		25.037 18.634 86.965 1.00 93.86	Ο
ATOM			27.466 19.336 85.469 1.00 97.13	С
ATOM		CG TYR B 331	27.069 20,568 86.213 1.00101.71	С
	2060	CD1 TYR B 331	26.608 21.704 85.561 1.00103.32	C
		CD2 TYR B 331	27.178 20.619 87.608 1.00104.18	C
		CE1 TYR B 331	26.226 22.828 86.263 1.00105.97	С
		CE2 TYR B 331	26.828 21.752 88.324 1.00106.55	C
		CZ TYR B 331	26,347 22,858 87.642 1.00107.31	С
ATOM		OH TYR B 331	25.995 24.000 88.323 1.00107.29	0
		N ALA B 340	39.286 16.946 89.923 1.00 93.98	N
		<b>CA ALA B 340</b>	38.917 16.738 88.521 1.00 93.62	С
		C ALA B 340	37.402 16.787 88.327 1.00 90.09	С
ATOM			36,868 16,237 87,370 1,00 90,38	0
		CB ALA B 340	39.519 15.472 87.926 1.00 94.53	С
		N SER B 341	36.706 17.458 89.239 1.00 85.89	N
		CA SER B 341	35.276 17.676 89.073 1.00 82.06	С
ATOM		C SER B 341	35.174 18.844 88.061 1.00 78.61	С
ATOM			34.785 18.752 86.908 1.00 80.07	0
		CB SER B 341	34.610 18.188 90.341 1.00 83.38	С

ATOM	2076	OG SER B 341	35.256 19.414 90.728 1.00 85.02	Ο
ATOM	2077	N MET B 342	35.722 19.964 88.528 1.00 71.83	N
<b>ATOM</b>	2078	CA MET B 342	35.738 21.170 87.702 1.00 67.11	С
<b>ATOM</b>	2079	C MET B 342	36.582 20.918 86.469 1.00 62.56	С
<b>ATOM</b>	2080	O MET B 342	36.233 21.329 85.369 1.00 62.00	0
<b>ATOM</b>	2081	CB MET B 342	36.320 22.295 88.511 1.00 71.06	С
<b>ATOM</b>	2082	CG MET B 342	36.550 23.547 87.695 1.00 76.61	С
<b>ATOM</b>	2083	SD MET B 342	36.328 24.989 88.764 1.00 82.30	S
<b>ATOM</b>	2084	CE MET B 342	37.859 25.853 88.353 1.00 81.45	С
<b>ATOM</b>	2085	N MET B 343	37.682 20.186 86.669 1.00 58.18	N
<b>ATOM</b>	2086	CA MET B 343	38.521 19.887 85.520 1.00 57.17	С
ATOM	2087	C MET B 343	37.765 18.915 84.625 1.00 53.51	С
ATOM		O MET B 343	37.989 18.950 83.422 1.00 54.37	0
ATOM		CB MET B 343	39.915 19.428 85.885 1.00 60.29	С
ATOM			40.925 20.583 85.969 1.00 64.87	С
ATOM			40.885 21.649 84.487 1.00 70.97	S
ATOM		CE MET B 343	41.239 20.401 83.224 1.00 67.55	С
ATOM		N GLY B 344	36.877 18.128 85.204 1.00 50.03	N
ATOM			36.100 17.109 84.489 1.00 45.01	С
ATOM		C GLY B 344	35.089 17.784 83.576 1.00 44.23	C
ATOM		O GLY B 344	35.007 17.591 82.362 1.00 44.89	0
ATOM		N LEUB 345	34.395 18.715 84.226 1.00 41.93	N
ATOM		CA LEU B 345	33.397 19.513 83.562 1.00 42.59	С
ATOM		C LEUB 345	33.964 20.248 82.346 1.00 43.04	C
ATOM		O LEUB 345	33.393 20.250 81.229 1.00 40.37	0
ATOM		CB LEUB 345	32.765 20.451 84.561 1.00 43.09	C
ATOM		CG LEUB 345		C
ATOM			30.750 21.109 85.884 1.00 42.87	C
		CD2 LEU B 345	30.825 18.815 84.964 1.00 43.41	C
		N LEUB 346	35.112 20.870 82.544 1.00 41.05	N
		CA LEUB 346	35.738 21.616 81.445 1.00 40.63	C
ATOM		C LEUB 346		C
ATOM		O LEUB 346	36.259 21.034 79.158 1.00 38.60	0
		CB LEUB 346	36.802 22.539 82.083 1.00 40.84	C
		CG LEU B 346 CD1 LEU B 346	36.140 23.535 83.040 1.00 40.19 37.202 24.319 83.759 1.00 40.76	C
		CD1 LEU B 346 CD2 LEU B 346	35.106 24.415 82.336 1.00 37.83	C
		N THR B 347	36.709 19.510 80.739 1.00 38.21	N
		CA THR B 347	37.285 18.607 79.711 1.00 38.77	C
		C THR B 347	36.175 18.060 78.878 1.00 38.77	c
ATOM			36.273 17.880 77.679 1.00 41.54	Ö
		CB THR B 347	38.055 17.505 80.445 1.00 35.92	C
		OG1 THR B 347	38.933 17.303 80.443 1.00 33.92	o
		CG2 THR B 347	38.918 16.662 79.577 1.00 35.35	C
		N ASN B 348	35.066 17.774 79.565 1.00 42.21	N
		CA ASN B 348	33,930 17,197 78.816 1.00 40.77	C
		C ASN B 348	33.447 18.316 77.893 1.00 37.78	c
ATOM			33.306 18.016 76.707 1.00 41.02	Ö
ATOM		CB ASN B 348	32.835 16.674 79.718 1.00 46.33	Č
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33.266 27.248 62.885 1.00 31.31 C ATOM 2223 CG TRP B 360 ATOM 2224 CD1 TRP B 360 32.726 28.432 62.489 1.00 30.14 C 34.656 27.477 63.095 1.00 27.29 ATOM 2225 CD2 TRP B 360 33.690 29.405 62.477 1.00 28.74 ATOM 2226 NE1 TRP B 360 34.887 28.837 62.861 1.00 28.25 C ATOM 2227 CE2 TRP B 360 C ATOM 2228 CE3 TRP B 360 35.721 26.680 63.511 1.00 28.20 C 36.130 29.430 63.024 1.00 24.96 ATOM 2229 CZ2 TRP B 360 C ATOM 2230 CZ3 TRP B 360 36.960 27.283 63.666 1.00 27.77 37,152 28,642 63,395 1.00 25,71 ATOM 2231 CH2 TRP B 360 34.937 24.709 61.298 1.00 39.67 N ATOM 2232 N ALA B 361 C 36.185 24.796 60.527 1.00 43.20 ATOM 2233 CA ALA B 361 35.935 24.626 59.036 1.00 42.09 C ATOM 2234 C ALA B 361 ATOM 2235 O ALA B 361 36.251 25.465 58.184 1.00 37.43 0 ATOM 2236 CB ALA B 361 37.143 23.729 61.106 1.00 42.72 C 35.254 23.526 58.685 1.00 43.79 ATOM 2237 N LYS B 362 N ATOM 2238 CA LYS B 362 34.880 23.171 57.339 1.00 44.31 34.013 24.211 56.671 1.00 43.19 C ATOM 2239 C LYS B 362 ATOM 2240 O LYS B 362 33.967 24.256 55.448 1.00 46.74 34.254 21.793 57.234 1.00 44.89 C ATOM 2241 CB LYS B 362 C ATOM 2242 CG LYS B 362 35.116 20.662 57.747 1.00 47.52 C 36.192 20.357 56.692 1.00 53.22 ATOM 2243 CD LYS B 362 C ATOM 2244 CE LYS B 362 36.618 18.891 56.666 1.00 55.05 N ATOM 2245 NZ LYS B 362 37.853 18.714 55.815 1.00 58.66 ATOM 2246 N ARG B 363 33.436 25.182 57.330 1.00 44.77 N ATOM 2247 CA ARG B 363 32.688 26.238 56.688 1.00 46.46 C ATOM 2248 C ARG B 363 33.447 27.545 56.666 1.00 47.06 32.952 28.594 56.190 1.00 47.77 0 ATOM 2249 O ARG B 363 31.285 26.352 57.252 1.00 51.47 ATOM 2250 CB ARG B 363 30.599 24.978 57.257 1.00 57.74 ATOM 2251 CG ARG B 363 C 29.144 25.078 57.571 1.00 63.24 ATOM 2252 CD ARG B 363 ATOM 2253 NE ARG B 363 28.714 24.274 58.675 1.00 72.16 ATOM 2254 CZ ARG B 363 27.641 24.366 59.454 1.00 77.17 ATOM 2255 NH1 ARG B 363 26.690 25.290 59.359 1.00 78.21 N ATOM 2256 NH2 ARG B 363 27.503 23.448 60.423 1.00 78.39 N 34.701 27.524 57.115 1.00 43.37 N ATOM 2257 N VAL B 364 35,437 28,786 56,962 1.00 46.62 C ATOM 2258 CA VAL B 364 C ATOM 2259 C VAL B 364 35.978 28.824 55.552 1.00 51.16 36.718 27.947 55.063 1.00 53.83 0 ATOM 2260 O VAL B 364 36.455 28.883 58.101 1.00 45.62 ATOM 2261 CB VAL B 364 ATOM 2262 CG1 VAL B 364 37.501 29.930 57.814 1.00 40.24 C 35,697 29,179 59,395 1.00 41.67 ATOM 2263 CG2 VAL B 364 ATOM 2264 N PRO B 365 35.581 29.804 54.781 1.00 54.29 N 36.002 30.007 53.408 1.00 54.11 С ATOM 2265 CA PRO B 365 37.505 29.941 53.286 1.00 56.48 С ATOM 2266 C PRO B 365 38.258 30.675 53.911 1.00 57.71 0 ATOM 2267 O PRO B 365 ATOM 2268 CB PRO B 365 35.484 31.391 52.999 1.00 55.74 C ATOM 2269 CG PRO B 365 34.239 31.482 53.865 1.00 56.60 C ATOM 2270 CD PRO B 365 34.660 30.870 55.221 1.00 57.46 C ATOM 2271 N GLY B 366 37.968 28.989 52.492 1.00 59.01 N

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ATOM	2272	CA GLY B 366	39.367 28.719 52.206 1.00 56.53	С
<b>ATOM</b>	2273	C GLY B 366	39.814 27.449 52.896 1.00 56.39	C
<b>ATOM</b>	2274	O GLY B 366	40.701 26.721 52.453 1.00 57.87	Ο
<b>ATOM</b>	2275	N PHE B 367	39.185 27.178 54.044 1.00 54.29	N
<b>ATOM</b>	2276	CA PHE B 367	39.568 26.030 54.829 1.00 51.31	С
ATOM	2277	C PHE B 367	39.509 24.725 54.071 1.00 51.54	С
ATOM	2278	O PHE B 367	40.379 23.888 54.307 1.00 55.10	0
ATOM	2279	CB PHE B 367	38.689 25.855 56.102 1.00 45.65	С
ATOM	2280	CG PHE B 367	39.438 24.995 57.091 1.00 41.76	С
ATOM	2281	CD1 PHE B 367	40.589 25.494 57.707 1.00 40.04	С
ATOM	2282	CD2 PHE B 367	39.023 23.713 57.375 1.00 38.51	С
ATOM	2283	CE1 PHE B 367	41.273 24.731 58.636 1.00 37.07	С
ATOM	2284	<b>CE2 PHE B 367</b>	39.717 22.963 58.321 1.00 36.35	С
ATOM	2285	CZ PHE B 367	40.834 23.460 58.936 1.00 33.86	С
ATOM	2286	N VAL B 368	38.474 24.480 53.298 1.00 52.13	N
		CA VAL B 368	38,363 23,114 52,736 1.00 54.30	С
		C VAL B 368	39.143 22.975 51.486 1.00 57.80	С
ATOM		O VAL B 368	39.401 21.869 50.998 1.00 63.60	0
ATOM	2290	CB VAL B 368	36,907 22.637 52.764 1.00 53.61	С
ATOM	2291	CG1 VAL B 368	36.182 22.937 51.495 1.00 47.24	С
ATOM	2292	<b>CG2 VAL B 368</b>	36,822 21,182 53,236 1,00 53,23	С
ATOM	2293	N ASP B 369	39.682 24.036 50.920 1.00 59.22	N
ATOM	2294	CA ASP B 369		C
ATOM	2295	C ASP B 369	41.975 23.618 50.187 1.00 61.08	С
		O ASP B 369	42.917 23.513 49.408 1.00 65.57	0
ATOM	•	CB ASP B 369	40.764 25.614 49.507 1.00 60.75	С
ATOM	2298	CG ASP B 369	39.544 26.116 48.756 1.00 62.62	С
ATOM	2299	OD1 ASP B 369	38.792 25.215 48.325 1.00 64.13	. 0
ATOM	2300	OD2 ASP B 369	39.395 27.336 48.564 1.00 62.51	0
ATOM	2301	N LEUB 370	42.173 23.356 51.457 1.00 57.11	N
ATOM	2302	CA LEUB 370	43,421 22,936 51,990 1.00 56,49	С
ATOM	2303	C LEU B 370	43.455 21.412 52.023 1.00 57.13	С
ATOM	2304	O LEU B 370	42,388 20.842 52.060 1.00 59.40	0
		CB LEUB 370	43,514 23,456 53,430 1.00 55,70	С
		CG LEUB 370	43,789 24,926 53,676 1.00 52,48	С
ATOM	2307	CD1 LEU B 370	44.811 25.033 54.778 1.00 52.72	С
ATOM	2308	CD2 LEU B 370	44,290 25.641 52.439 1.00 54.40	С
		N THR B 371	44.648 20.857 52.022 1.00 56.95	N
ATOM	2310	CA THR B 371	44.804 19.440 52.137 1.00 57.71	С
<b>ATOM</b>	2311	C THR B 371	44.344 19.082 53.556 1.00 58.84	С
ATOM			44.392 19.912 54.471 1.00 58.64	0
		CB THR B 371	46.257 18.949 51.967 1.00 59.95	С
<b>ATOM</b>	2314	OG1 THR B 371	47.063 19.177 53.118 1.00 58.30	O
ATOM	2315	CG2 THR B 371	46,924 19.573 50.745 1.00 60.40	С
		N LEUB 372	43.993 17.828 53.732 1.00 60.21	N
		CA LEUB 372	43.598 17.318 55.034 1.00 62.03	С
		C LEU B 372	44.728 17.567 56.026 1.00 63.78	С
		O LEUB 372	44.474 18.069 57.134 1.00 66.06	0
		CB LEUB 372	43.218 15.852 54.890 1.00 62.64	С

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			42.780 15.076 56.117 1.00 66.44	C
			41.896 15.921 57.053 1.00 64.82	C
			42.018 13.815 55.715 1.00 67.73	С
			45.992 17.295 55.677 1.00 64.79	N
			47.067 17.517 56.603 1.00 66.99	С
		C HIS B 373		С
			47.443 19.187 58.196 1.00 59.54	0
<b>ATOM</b>	2328	CB HIS B 373	48.496 17.289 56.089 1.00 76.41	С
			48.547 15.901 55.537 1.00 87.82	С
<b>ATOM</b>	2330	ND1 HIS B 373	47.917 14.825 56.131 1.00 89.75	N
<b>ATOM</b>	2331	CD2 HIS B 373	49.156 15.441 54.408 1.00 93.11	С
<b>ATOM</b>	2332	CE1 HIS B 373	48.126 13.744 55.408 1.00 92.37	С
<b>ATOM</b>	2333	<b>NE2 HIS B 373</b>	48.876 14.081 54.357 1.00 95.93	N
<b>ATOM</b>	2334	N ASP B 374	46.952 19.840 56.063 1.00 55.09	N
<b>ATOM</b>	2335	CA ASP B 374	46.990 21.246 56.394 1.00 53.61	С
<b>ATOM</b>	2336	C ASP B 374	45.862 21.661 57.317 1.00 52.72	C
<b>ATOM</b>	2337	O ASP B 374	46.101 22.487 58.199 1.00 52.25	0
<b>ATOM</b>	2338	CB ASP B 374	46.929 22.068 55.120 1.00 56.95	С
			48.340 22.005 54.524 1.00 58.90	С
			49.234 21.611 55.307 1.00 59.70	0
			48.382 22.331 53.335 1.00 60.88	0
			44.696 21.062 57.078 1.00 48.20	N
			43.547 21.361 57.929 1.00 44.27	С
			43.825 20.918 59.341 1.00 42.91	С
			43.586 21.609 60.327 1.00 44.49	Ο
		CB GLN B 375		С
			41.962 21.403 55.992 1.00 42.71	С
		CD GLN B 375		С
		OE1 GLN B 375		Ο
		<b>NE2 GLN B 375</b>		N
ATOM	2351	N VAL B 376	44.428 19.771 59.518 1.00 42.38	N
		CA VALB 376		С
		C VAL B 376		C
		O VAL B 376	45.836 20.342 62.711 1.00 48.81	0
		<b>CB VAL B 376</b>	45.295 17.844 60.678 1.00 39.53	C
		CG1 VAL B 376	45.791 17.269 61.958 1.00 37.82	C
		CG2 VAL B 376	44.319 16.979 59.903 1.00 37.59	С
		N HISB 377	46.740 20.644 60.667 1.00 44.81	N
		CA HIS B 377	47.792 21.478 61.269 1.00 44.39	С
		C HIS B 377	47.155 22.780 61.769 1.00 41.44	C
		O HIS B 377	47.358 23.208 62.881 1.00 42.24	0
		CB HIS B 377	48.970 21.761 60.372 1.00 41.82	С
		N LEUB 378	46.287 23.384 60.995 1.00 38.79	N
		CA LEUB 378	45.586 24.560 61.452 1.00 37.49	C
		C LEUB 378	44.817 24.307 62.738 1.00 39.70	C
		O LEUB 378	44.965 25.065 63.742 1.00 40.23	0
		CB LEUB 378	44.792 25.084 60.278 1.00 34.49	· C
		CG LEUB 378	45.660 25.626 59.142 1.00 33.30	C
ATOM	2374	CD1 LEU B 378	44.776 26.268 58.061 1.00 35.31	С

	2375 CD2 LEU B 378	46.652 26.648 59.629 1.00 31.86	С
ATOM	2376 N LEUB 379	44.014 23.264 62.855 1.00 39.55	N
ATOM	2377 CA LEU B 379	43.281 23.045 64.108 1.00 39.47	С
<b>ATOM</b>	2378 C LEUB 379	44.236 22.621 65.183 1.00 40.67	С
ATOM	2379 O LEUB 379	44.113 22.953 66.367 1.00 44.03	0
<b>ATOM</b>	2380 CB LEU B 379	42.165 22.022 63.905 1.00 36.04	С
<b>ATOM</b>	2381 CG LEU B 379	41.035 22.590 63.044 1.00 36.14	С
<b>ATOM</b>	2382 CD1 LEU B 379	40.367 21.487 62.267 1.00 35.56	С
<b>ATOM</b>	2383 CD2 LEU B 379	40.005 23.346 63.905 1.00 35.13	С
<b>ATOM</b>	2384 N GLUB 380	45.299 21.916 64.808 1.00 44.30	N
<b>ATOM</b>	2385 CA GLU B 380	46.131 21.413 65.904 1.00 47.28	С
<b>ATOM</b>	2386 C GLUB 380	46.648 22.562 66.732 1.00 46.23	С
<b>ATOM</b>	2387 O GLUB 380	46.674 22.437 67.945 1.00 47.50	0
<b>ATOM</b>	2388 CB GLUB 380	47.223 20.484 65.491 1.00 55.36	C
<b>ATOM</b>	2389 CG GLU B 380	47.687 19.578 66.656 1. <b>00 62.14</b>	С
ATOM	2390 CD GLU B 380	48.998 18.908 66.279 1.00 68.73	С
ATOM	2391 OE1 GLU B 380	49.450 19.015 65.098 1.00 70.64	0
ATOM	2392 OE2 GLU B 380	49.588 18.269 67.182 1.00 73.27	0
ATOM	2393 N CYS B 381	47.067 23.599 66.056 1.00 45.88	N
ATOM	2394 CA CYS B 381	47.624 24.810 66.658 1.00 44.73	С
ATOM	2395 C CYS B 381	46.566 25.784 67.130 1.00 42.92	C
ATOM	2396 O CYS B 381	46.792 26.395 68.178 1.00 37.98	0
ATOM	2397 CB CYS B 381	48.572 25.454 65.635 1.00 52.09	С
<b>ATOM</b>	2398 SG CYS B 381	50.273 25.860 66.085 1.00 62.86	S
<b>ATOM</b>	2399 N ALA B 382	45.379 25.940 66.551 1.00 40.58	N
<b>ATOM</b>	2400 CA ALA B 382	44.429 26.942 66.967 1.00 38.93	С
<b>ATOM</b>	2401 C ALA B 382	43.279 26.563 67.872 1.00 38.58	C
<b>ATOM</b>	2402 O ALA B 382	42.620 27.427 68.424 1.00 37.32	0
<b>ATOM</b>	2403 CB ALA B 382	43.707 27.386 65.671 1.00 38.68	С
<b>ATOM</b>	2404 N TRP B 383	43.028 25.289 68.081 1.00 38.92	N
<b>ATOM</b>	2405 CA TRP B 383	41.892 24.847 68.875 1.00 36.09	С
<b>ATOM</b>	2406 C TRP B 383	41.683 25.516 70.178 1.00 35.26	С
<b>ATOM</b>	2407 O TRP B 383	40.574 26.008 70.530 1.00 33.42	0
	2408 CB TRP B 383	41.904 23.306 68.816 1.00 35.35	C.
	2409 CG TRP B 383	42.837 22.774 69.826 1.00 33.79	C
	2410 CD1 TRP B 383	44.153 22.436 69.663 1.00 34.99	C
	2411 CD2 TRP B 383	42.517 22.560 71.200 1.00 32.33	С
	2412 NE1 TRP B 383	44.662 22.021 70.857 1.00 30.51	N
	2413 CE2 TRP B 383	43.696 22.081 71.823 1.00 29.75	C
	2414 CE3 TRP B 383	41.355 22.750 71.944 1.00 30.48	C
	2415 CZ2 TRP B 383		C
	2416 CZ3 TRP B 383	41.383 22.455 73.268 1.00 31.00	C
	2417 CH2 TRP B 383	42.591 21.963 73.857 1.00 33.85	С
	2418 N LEUB 384	42.744 25.635 70.972 1.00 33.40	N
	2419 CA LEUB 384	42.585 26.325 72.255 1.00 30.50	C
	2420 C LEUB 384	42.335 27.795 72.058 1.00 31.57	C
	2421 O LEUB 384	41.532 28.347 72.806 1.00 35.39	0
	2422 CB LEUB 384	43.720 26.041 73.207 1.00 26.71	C
ATOM	2423 CG LEUB 384	43.548 26.567 74.605 1.00 30.98	С

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ΔΤΟΜ	2424	CDLIFUR 384	42.142 26.159 75.119 1.00 28.22	С
			44.636 26.068 75.544 1.00 30.47	
		N GLUB 385		
			42.672 29.904 70.872 1.00 31.19	
ATOM	2428	C GLU B 385	41.220 30.055 70.463 1.00 33.31	С
			40.514 31.029 70.802 1.00 37.28	
ATOM	2430	CB GLUB 385	43.519 30.540 69.811 1.00 33.75 45.019 30.277 69.811 1.00 38.27	С
ATOM	2431	CG GLU B 385	45.019 30.277 69.811 1.00 38.27	С
<b>ATOM</b>	2432	CD GLUB 385	45.821 31.092 68.845 1.00 37.52	С
ATOM	2433	OE1 GLU B 385	45.581 32.266 68.657 1.00 39.60	O
ATOM	2434	OE2 GLU B 385	46.769 30.620 68.199 1.00 44.18	0
			40.737 29.029 69.767 1.00 32.56	N
			39.318 29.081 69.346 1.00 32.62	
			38.361 28.909 70.500 1.00 30.09	
ATOM	2438	O ILE B 386	37.359 29.606 70.692 1.00 25.95	0
			39.100 28.108 68.191 1.00 33.30	
			39.894 28.679 66.969 1.00 34.06	
ATOM	2441	CG2 ILE B 386	37.643 28.026 67.815 1.00 34.81	C
ATOM	2442	CD1 ILE B 386	39.864 27.634 65.882 1.00 37.55 38.667 27.956 71.384 1.00 27.87	С
			37.825 27.773 72.542 1.00 26.27	
			37.817 29.048 73.365 1.00 29.90	
ATOM	2446	O LEUB 387	36.749 29.493 73.824 1.00 27.72	0
ATOM	2447	CB LEUB 387	38.375 26.590 73.322 1.00 23.50	C C
			37.930 25.215 72.829 1.00 26.32	
			38.303 24.168 73.896 1.00 21.89 36.426 25.150 72.471 1.00 21.80	
ATOM	2450	N MET D 200	39.039 29.641 73.530 1.00 32.23	
ATOM	2431	CA WELD 366	39.121 30.826 74.393 1.00 31.87	C
			38.427 32.009 73.806 1.00 31.46	
		O MET B 388		Ö
			40.499 31.143 74.859 1.00 31.50	C
			41.227 30.030 75.631 1.00 32.92	Č
			42.970 30.484 75.860 1.00 33.47	S
			43.587 29.273 76.951 1.00 27.60	Č
		N ILE B 389	38.672 32.264 72.523 1.00 30.09	N
		CA ILE B 389	37.966 33.444 71.987 1.00 25.61	C
		C ILE B 389	36,495 33,253 72,136 1.00 28,80	С
		O ILE B 389	35.793 34.263 72.389 1.00 34.46	0
<b>ATOM</b>	2463	CB ILE B 389	38.481 33.851 70.625 1.00 24.14	С
ATOM	2464	CG1 ILE B 389	38.357 35.373 70.508 1.00 25.05	С
ATOM	2465	CG2 ILE B 389	37.936 33.063 69.481 1.00 19.98	С
			38.059 35.936 69.168 1.00 28.34	С
		N GLY B 390	35.932 32.076 72.040 1.00 30.54	N
ATOM	2468	CA GLY B 390	34.488 31.888 72.191 1.00 33.74	С
		C GLY B 390	34.072 32.112 73.639 1.00 37.29	С
			33.044 32.716 73.939 1.00 36.80	0
		N LEUB 391		N
ATOM	2472	CA LEU B 391	34.604 31.848 75.994 1.00 35.83	С

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ATOM	2473 C LEUB 391	34.570 33.325 76.242 1.00 34.46	С
ATOM		33.700 33.918 76.805 1.00 33.17	О
ATOM		35.734 31.153 76.794 1.00 31.89	С
ATOM		35.804 31.397 78.283 1.00 31.45	С
	2477 CD1 LEU B 391	34.434 31.098 78.962 1.00 27.42	C
	2478 CD2 LEU B 391	36.881 30.540 78.949 1.00 <b>28.7</b> 5	C
	2479 N VAL B 392		N
	2480 CA VAL B 392	35.682 35.420 75.958 1.00 35.50	C
	2481 C VAL B 392	34.427 36.097 75.475 1.00 34.25	C
	2482 O VAL B 392		Ö
	2483 CB VAL B 392	36.940 36.027 75.296 1.00 36.25	C
ATOM		36.823 37.540 75.354 1.00 37.18	C
ATOM		38.161 35.626 76.107 1.00 35.78	Č
	2486 N TRP B 393	34.037 35.771 74.253 1.00 37.03	N
	2487 CA TRP B 393		c
		31.642 36.272 74.423 1.00 40.00	c
ATOM		30.896 37.192 74.710 1.00 42.71	Ö
ATOM		32.740 35.936 72.209 1.00 37.68	c
ATOM			Č
ATOM		30.405 35.350 71.438 1.00 38.63	C
ATOM		30.971 37.487 71.102 1.00 35.68	Č
	2493 CD2 TRP B 393	29.324 36.007 70.826 1.00 41.40	N
	2494 NE1 TRP B 393		C
	2495 CE2 TRP B 393	29.678 37.308 70.602 1.00 37.07	C
	2496 CE3 TRP B 393	31.542 38.740 70.957 1.00 36.83	C
ATOM	2497 CZ2 TRP B 393	28.961 38.338 70.031 1.00 36.96	C
ATOM		30.857 39.743 70.349 1.00 33.97	C
ATOM		29.553 39.557 69.920 1.00 34.11	N
ATOM		31.366 35.039 74.802 1.00 39.93	C
ATOM	2501 CA ARG B 394	30.174 34.701 75.560 1.00 36.65	c
ATOM	2502 C ARG B 394		. 0
ATOM		. 29.194 35.311 77.694 1.00 41.96	
	2504 CB ARG B 394		C C
	2505 CG ARG B 394		C
	2506 CD ARG B 394		N
	2507 NE ARG B 394	30.928 29.919 76.189 1.00 28.98	C
	2508 CZ ARG B 394		N
ATOM	2509 NH1 ARG B 394	31.995 29.476 74.222 1.00 28.81	N
		32.703 28.414 76.192 1.00 26.10	N
	2511 N SER B 395	31.374 35.561 77.468 1.00 39.89	C
	2512 CA SER B 395	31.581 36.128 78.784 1.00 36.60	
	2513 C SER B 395	31.396 37.621 78.802 1.00 42.53	C
	2514 O SER B 395	31.142 38.237 79.847 1.00 46.22	0
	2515 CB SER B 395	33.039 35.845 79.155 1.00 31.85	C
	2516 OG SER B 395	33.079 34.457 79.436 1.00 28.12	O N
	2517 N MET B 396	31.520 38.302 77.688 1.00 47.19	N
	2518 CA MET B 396	31.421 39.733 77.641 1.00 51.47	C
	2519 C MET B 396	30.489 40.366 78.647 1.00 56.34	C
	2520 O MET B 396	30.895 41.118 79.524 1.00 60.12	0
ATOM	2521 CB MET B 396	30.902 40.139 76.254 1.00 49.14	С

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ATOM	2522 CG MET B 39	•	С
		31.548 41.224 73.856 1.00 42.86	
		30.173 40.085 73.579 1.00 50.12	
ATOM	2525 N GLUB 397	29.212 40.096 78.533 1.00 60.93	N
		7 28.199 40.683 79.382 1.00 65.88	
		27.987 39.977 80.693 1.00 66.69	
ATOM	2528 O GLUB 397	26.865 39.933 81.243 1.00 69.14	0
		26.895 40.725 78.560 1.00 68.52	
		7 27.191 41.201 77.117 1.00 70.94	
		29.052 39.472 81.294 1.00 63.21	
		29.084 38.799 82.562 1.00 62.64	
	2536 C HIS B 398		С
		31.215 38.369 83.640 1.00 64.14	O
<b>ATOM</b>	2538 CB HIS B 398	29.047 37.286 82.440 1.00 61.15	С
<b>ATOM</b>	2539 CG HIS B 398	27.721 36.747 82.061 1.00 63.91	С
<b>ATOM</b>	2540 ND1 HIS B 398	3 27.211 36.810 80.779 1.00 67.22	N
		26.766 36.129 82.765 1.00 65.22	
ATOM	2542 CE1 HIS B 398	26.028 36.256 80.685 1.00 65.18	С
ATOM	2543 NE2 HIS B 398	25.756 35.822 81.899 1.00 66.32	N
		30.569 40.505 83.387 1.00 63.39	
		31.751 41.084 83.999 1.00 62.77	
		32.046 40.395 85.316 1.00 62.99	
		31.131 40.222 86.121 1.00 66.99	
		31.512 42.569 84.233 1.00 64.41	
		30.077 42.748 83.819 1.00 65.85	
		29.632 41.547 83.014 1.00 64.17	
		33.283 40.001 85.491 1.00 60.52	
		33.805 39.350 86.646 1.00 58.08 33.773 37.854 86.557 1.00 59.78	
		34.357 37.126 87.369 1.00 60.70	
		33.025 37.335 85.584 1.00 61.41	
		32.870 35.896 85.450 1.00 61.48	
		33.127 35.416 84.033 1.00 56.79	
		32.888 36.166 83.100 1.00 57.78	
		31.394 35.554 85.812 1.00 68.06	
		31.103 35.685 87.314 1.00 72.86	
		29.880 34.879 87.707 1.00 77.25	
		29.705 34.764 89.220 1.00 79.35	
ATOM	2563 NZ LYS B 401	29.631 33.337 89.702 1.00 80.08	N
<b>ATOM</b>	2564 N LEUB 402	33.544 34.179 83.889 1.00 49.79	N
		33.670 33.432 82.678 1.00 42.60	
ATOM	2566 C LEUB 402	32.478 32.509 82.437 1.00 41.15	С
	2567 O LEUB 402		
		2 34.960 32.546 82.682 1.00 33.63	
		2 36.184 33.473 82.725 1.00 32.31	
		2 37.502 32.732 82.793 1.00 23.92	
		2 36.090 34.463 81.577 1.00 30.62	
		31.775 32.667 81.328 1.00 39.54	
ATOM	2573 CA LEUB 403	30.640 31.792 81.035 1.00 39.78	С

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ATOM	2574 C LEUB 403		C
ATOM		30.816 30.480 78.966 1.00 39.71	0
ATOM		29.533 32.667 80.452 1.00 42.24	C
ATOM	2577 CG LEUB 403		C
ATOM	2578 CD1 LEU B 403	27.362 31.660 81.021 1.00 45.14	C
ATOM	2579 CD2 LEU B 403	27.562 32.874 78.861 1.00 43.05	C
ATOM	2580 N PHE B 404	31.718 29.626 80.832 1.00 40.77	N
ATOM	2581 CA PHE B 404		С
ATOM	2582 C PHE B 404	30.962 27.790 79.501 1.00 40.29	C
ATOM	2583 O PHE B 404		0
ATOM		32,905 27.438 81.026 1.00 37.12	C
ATOM			C
ATOM	2586 CD1 PHE B 404	34.333 28.785 82.593 1.00 35.02	C
		35.395 27.576 80.848 1.00 31.59	C
ATOM		35.587 29.241 83.023 1.00 37.43	C
ATOM		36.616 28.005 81.263 1.00 30.58	C
ATOM		36.740 28.838 82.341 1.00 33.26	С
ATOM		29.828 27.789 80.137 1.00 41.67	N
ATOM	•	28.558 27.337 79.623 1.00 39.74	С
ATOM	2593 C ALA B 405		C
ATOM		27.723 28.829 81.314 1.00 45.02	0
ATOM	2595 CB ALA B 405		С
	2596 N PRO B 406		N
	2597 CA PRO B 406	25.134 28.819 80.323 1.00 39.78	С
ATOM	2598 C PRO B 406	24.922 28.230 81.704 1.00 43.39	C
ATOM	2599 O PRO B 406	24.687 28.978 82.635 1.00 47.07	0
ATOM	2600 CB PRO B 406	· ·	C
ATOM	2601 CG PRO B 406		C
ATOM	2602 CD PRO B 406	25.913 27.404 78.549 1.00 40.30	C
ATOM	2603 N ASN B 407		N
ATOM		24.938 26.334 83.217 1.00 44.35	C
ATOM			C
ATOM	2606 O ASN B 407	26.358 25.322 84.859 1.00 43.21	0
	2607 CB ASN B 407	24.207 24.990 83.095 1.00 45.30	C
	2608 CG ASN B 407	25.102 23.905 82.560 1.00 48.52	C
	2609 OD1 ASN B 407	26.017 24.173 81.765 1.00 52.75	0
	2610 ND2 ASN B 407	24.868 22.682 82.982 1.00 47.55	N
	2611 N LEUB 408	27.230 26.971 83.581 1.00 44.78	N
	2612 CA LEUB 408	28.530 26.840 84.245 1.00 43.66	C
	2613 C LEUB 408	29.274 28.160 84.105 1.00 46.96	C
	2614 O LEUB 408	30.177 28.206 83.300 1.00 47.50	0
	2615 CB LEUB 408	29.348 25.734 83.640 1.00 39.42	C
	2616 CG LEUB 408	30.702 25.450 84.231 1.00 41.46	C
	2617 CD1 LEUB 408	30.579 25.028 85.691 1.00 43.35	C
	2618 CD2 LEU B 408	31.454 24.396 83.439 1.00 40.80	C
	2619 N LEU B.409	28.857 29.155 84.856 1.00 49.18	N
ATOM		29.399 30.474 84.971 1.00 51.85	C
ATOM		30.384 30.538 86.149 1.00 54.53	C
ATOM	2622 O LEUB 409	29.967 30.547 87.300 1.00 57.83	0

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ATOM			С
ATOM	2673 C GLY B 415	40.291 29.004 89.616 1.00 <b>87</b> .99	С
ATOM	2674 O GLY B 415	41.156 28.238 89.181 1.00 86.24	O
ATOM	2675 N LYS B 416	40.364 29.509 90.842 1.00 90.55	N
ATOM	2676 CA LYS B 416	41.442 29.218 91.767 1.00 93.58	С
ATOM	2677 C LYS B 416	41.561 27.754 92.141 1.00 95.38	С
ATOM	2678 O LYS B 416	42.671 27.241 92.349 1.00 95.66	Ο
ATOM	2679 CB LYS B 416	41.269 30.074 93.037 1.00 93.15	С
<b>ATOM</b>	2684 N CYS B 417	40.489 26.977 92.152 1.00 97.58	N
<b>ATOM</b>	2685 CA CYS B 417	40.448 25.571 92.472 1.00100.45	С
<b>ATOM</b>	2686 C CYS B 417	41.276 24.692 91.543 1.00 99.99	С
<b>ATOM</b>	2687 O CYS B 417	41.292 23.457 91.586 1.00 99.87	0
<b>ATOM</b>	2688 CB CYS B 417	39.005 25.045 92.445 1.00103.57	С
<b>ATOM</b>	2689 SG CYS B 417	37.717 25.947 93.323 1.00109.90	S
<b>ATOM</b>	2690 N VALB 418	41.992 25.273 90.607 1.00 99.92	N
ATOM	2691 CA VALB 418	42.857 24.622 89.651 1.00 99.16	С
ATOM	2692 C VAL B 418	44.197 25.380 89.670 1.00 98.34	С
<b>ATOM</b>	2693 O VAL B 418	44.186 26.600 89.508 1.00 97.73	0
<b>ATOM</b>	2694 CB VAL B 418	42.303 24.667 88.218 1.00 99.72	С
<b>ATOM</b>	2695 CG1 VAL B 418	43.007 23.621 87.358 1.00 97.84	С
ATOM	2696 CG2 VAL B 418	40.795 24.517 88.146 1.00 98.53	С
ATOM	2697 N GLUB 419	45.278 24.673 89.873 1.00 98.42	N
ATOM	2698 CA GLUB 419	46.605 25.274 89.952 1.00 98.68	С
ATOM	2699 C GLUB 419	47.104 25.893 88.661 1.00 97.48	Ċ
ATOM	2700 O GLUB 419	47.289 25.222 87.639 1.00 98.90	О
ATOM	2701 CB GLU B 419	47.598 24.230 90.490 1.00 99.66	С
ATOM	2706 N GLY B 420	47.362 27.207 88.696 1.00 94.17	N
ATOM	2707 CA GLY B 420	47.816 27.918 87.511 1.00 91.36	С
ATOM	2708 C GLY B 420	46.684 28.553 86.708 1.00 88.54	С
ATOM	2709 O GLY B 420	46.918 29.464 85.895 1.00 88.73	0
ATOM	2710 N MET B 421	45.435 28.140 86.958 1.00 83.23	N
ATOM	2711 CA MET B 421	44.336 28.679 86,203 1.00 80.10	С
ATOM	2712 C MET B 421	44.023 30.138 86.465 1.00 76.64	С
		43.546 30.845 85.548 1.00 77.79	0
	2714 CB MET B 421	43.107 27.781 86.353 1.00 80.33	С
	2715 CG MET B 421	42.062 28.036 85.275 1.00 79.26	С
		40.735 26.848 85.309 1.00 79.88	S
	2717 CE MET B 421	41.509 25.424 84.511 1.00 78.20	С
	2718 N VAL B 422	44.329 30.649 87.633 1.00 70.06	N
	2719 CA VAL B 422	44.014 32.028 87.971 1.00 66.93	С
	2720 C VAL B 422	44.617 33.051 87.034 1.00 62.98	С
	2721 O VAL B 422	43.970 33.990 86.582 1.00 59.44	0
	2722 CB VAL B 422	44.481 32.384 89.405 1.00 67.44	С
	2723 CG1 VAL B 422	43.588 33.465 89.994 1.00 66.70	С
	2724 CG2 VAL B 422	44.478 31.117 90.259 1.00 69.52	С
	2725 N GLUB 423	45.911 32.877 86.738 1.00 62.98	N
	2726 CA GLU B 423	46.561 33.863 85.854 1.00 60.72	С
	2727 C GLUB 423	45.900 33.831 84.486 1.00 56.94	С
ATOM	2728 O GLUB 423	45.496 34.892 83.976 1.00 58.86	О

			48.059 33.742 85.792 1.00 59.28	С
			45.629 32.636 83.964 1.00 50.05	N
			44.981 32.635 82.652 1.00 48.51	С
		C ILE B 424		С
			43.062 33.956 81.959 1.00 47.73	0
			45.041 31.288 81.951 1.00 44.17	С
<b>ATOM</b>	2739	CG1 ILE B 424	46.526 30.904 81.777 1.00 41.42	С
<b>ATOM</b>	2740	CG2 ILE B 424	44.420 31.454 80.588 1.00 40.80	С
<b>ATOM</b>	2741	CD1 ILE B 424	46.831 29.512 82.271 1.00 39.66	С
<b>ATOM</b>	2742	N PHE B 425	42.905 32.732 83.813 1.00 49.07	N
<b>ATOM</b>	2743	CA PHE B 425	41.562 33.166 84.131 1.00 49.17	С
<b>ATOM</b>	2744	C PHE B 425	41.450 34.686 84.190 1.00 49.03	С
ATOM	2745	O PHE B 425	40.517 35.354 83.723 1.00 46.73	0
<b>ATOM</b>	2746	CB PHE B 425	41.241 32.595 85.529 1.00 51.92	С
ATOM	2747	CG PHE B 425	39.762 32.392 85.709 1.00 51.58	С
ATOM	2748	CD1 PHE B 425	38.960 33.504 85.864 1.00 53.18	С
ATOM	2749	CD2 PHE B 425	39.212 31.134 85.713 1.00 50.30	С
ATOM	2750	CE1 PHE B 425	37.593 33.370 86.021 1.00 54.70	С
			37.858 30.966 85.875 1.00 51.75	С
<b>ATOM</b>	2752	CZ PHE B 425	37.049 32.078 86.029 1.00 54.42	С
ATOM	2753	N ASP B 426	42.475 35.304 84.790 1.00 48.98	N
<b>ATOM</b>	2754	CA ASP B 426	42.505 36.760 84.888 1.00 48.73	С
<b>ATOM</b>	2755	C ASP B 426	42.643 37.411 83.529 1.00 46.01	С
<b>ATOM</b>	2756	O ASP B 426	42.027 38.412 83.218 1.00 46.68	0
<b>ATOM</b>	2757	CB ASP B 426	43.708 37.168 85.736 1.00 52.22	С
<b>ATOM</b>	2758	CG ASP B 426	43.343 37.213 87.204 1.00 52.65	С
<b>ATOM</b>	2759	OD1 ASP B 426	42.139 37.339 87.499 1.00 54.85	Ο
<b>ATOM</b>	2760	OD2 ASP B 426	44.300 37.109 87.971 1.00 55.57	0
<b>ATOM</b>	2761	N MET B 427	43.495 36.795 82.730 1.00 44.72	N
<b>ATOM</b>	2762	CA MET B 427	43.797 37.174 81.364 1.00 41.75	С
<b>ATOM</b>	2763	C MET B 427	42.544 37.067 80.504 1.00 39.43	C
<b>ATOM</b>	2764	O MET B 427	42.155 37.984 79.789 1.00 39.81	Ο
<b>ATOM</b>	2765	CB MET B 427	44.907 36.188 80.884 1.00 44.36	С
<b>ATOM</b>	2766	CG MET B 427	46.294 36.729 81.084 1.00 48.85	С
<b>ATOM</b>	2767	SD MET B 427	47.678 35.780 80.492 1.00 55.91	S
<b>ATOM</b>	2768	CE MET B 427	47.419 34.154 81.133 1.00 52.49	C
<b>ATOM</b>	2769	N LEUB 428	41.814 35.942 80.690 1.00 35.14	N
<b>ATOM</b>	2770	CA LEUB 428	40.580 35.698 79.969 1.00 34.18	С
<b>ATOM</b>	2771	C LEU B 428	39.597 36.778 80.362 1.00 34.40	С
<b>ATOM</b>	2772	O LEUB 428	39.044 37.473 79.523 1.00 35.33	0
<b>ATOM</b>	2773	CB LEUB 428	39.989 34.299 80.162 1.00 30.49	С
<b>ATOM</b>	2774	CG LEUB 428	40.876 33.217 79.482 1.00 28.71	С
<b>ATOM</b>	2775	CD1 LEU B 428	40.714 31.829 79.995 1.00 26.98	С
<b>ATOM</b>	2776	CD2 LEU B 428	40.656 33.261 78.002 1.00 29.20	С
		N LEUB 429	39.562 37.071 81.667 1.00 37.03	N
		CA LEUB 429	38.678 38.138 82.109 1.00 35.92	С
		C LEU B 429	39.005 39.465 81.457 1.00 35.69	С
		O LEU B 429	38.047 40.111 80.996 1.00 33.54	O
		CB LEU B 429	38.703 38.277 83.621 1.00 32.15	С

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ATOM	2782	CG LEUB 429	37.830 37.222 84.321 1.00 33.08	С
		CD1 LEU B 429		C
		CD2 LEU B 429	36.362 37.329 83.909 1.00 29.01	Ċ
		N ALA B 430	40.296 39.813 81.393 1.00 32.95	N
		CA ALAB 430	40.634 41.126 80.826 1.00 36.84	C
		C ALA B 430	40,338 41.228 79.335 1.00 38.44	С
		O ALA B 430	39.968 42.264 78.761 1.00 36.45	0
		CB ALA B 430	42.102 41.541 81.010 1.00 34.40	С
		N THR B 431	40.580 40.079 78.661 1.00 37.54	N
ATOM	2791	CA THR B 431	40.159 40.081 77.252 1.00 36.70	С
ATOM	2792	C THR B 431	38.676 40.337 77.081 1.00 37.98	С
<b>ATOM</b>	2793	O THR B 431	38.287 41.142 76.201 1.00 35.69	Ο
<b>ATOM</b>	2794	CB THR B 431	40.645 38.754 76.682 1.00 35.10	С
ATOM	2795	OG1 THR B 431	42.064 38.624 77.003 1.00 38.56	0
<b>ATOM</b>	2796	CG2 THR B 431	40.434 38.713 75.188 1.00 31.41	С
ATOM	2797	N SER B 432	37.747 39.703 77.877 1.00 39.84	N
		CA SER B 432	36.344 39.976 77.574 1.00 45.36	С
ATOM	2799	C SER B 432	36.025 41.411 77.977 1.00 43.30	С
		O SER B 432	35.274 42.080 77.282 1.00 42.62	Ο
		CB SER B 432	35.225 39.117 78.140 1.00 45.94	С
		OG SER B 432	35.659 38.558 79.329 1.00 49.61	Ο
		N SER B 433	36.744 41.837 78.999 1.00 43.13	N
		CA SER B 433	36.535 43.234 79.330 1.00 46.73	С
		C SER B 433	36.855 44.133 78.146 1.00 46.01	С
		O SER B 433	36.086 45.008 77.734 1.00 49.24	0_
			37.281 43.646 80.573 1.00 49.56	C
			37.206 45.117 80.541 1.00 58.60	0
		N ARG B 434	37.992 43.977 77.531 1.00 45.21	N
		CA ARG B 434	38.409 44.760 76.382 1.00 44.15	C
		C ARG B 434	37.442 44.548 75.237 1.00 45.33	C
		O ARG B 434	37.074 45.482 74.494 1.00 45.12	0
			39.835 44.290 76.082 1.00 46.77	C
			40.513 45.050 74.967 1.00 55.03	C
			40.600 46.516 75.253 1.00 61.34	C
			40.638 47.463 74.192 1.00 66.92	N C
		CZ ARG B 434		
		NH1 ARG B 434	42.477 46.762 73.004 1.00 73.65 41.260 48.625 72.314 1.00 69.23	N N
		NH2 ARG B 434	36.897 43.321 75.074 1.00 69.23	N
		N PHE B 435	35.874 43.158 74.043 1.00 44.36	C
		CA PHE B 435		c
		O PHE B 435		Ö
			35,460 41.727 73,743 1.00 44.13	C
			36.410 40.882 72.948 1.00 46.42	Č
		CD1 PHE B 435	37.432 41.396 72.187 1.00 47.77	C
			36.310 39.505 72.955 1.00 48.65	Č
			38.314 40.645 71.467 1.00 46.44	Č
			37.178 38.706 72.249 1.00 50.86	Č
			38.196 39.278 71.493 1.00 49.02	Č
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ATOM	2831	N ARG B 436	34.265 44.140 75.618 1.00 45.66	N
ATOM	2832	CA ARG B 436	33.117 44.927 76.027 1.00 49.37	С
ATOM	2833	C ARG B 436	33.448 46.381 75.719 1.00 51.24	С
ATOM	2834	O ARG B 436	32.772 47.028 74.922 1.00 53.18	Ο
ATOM	2835	CB ARG B 436	32.757 44.830 77.483 1.00 52.16	С
ATOM	2836	CG ARG B 436	31.286 44.952 77.889 1.00 54.69	С
ATOM	2837	CD ARG B 436	31.216 44.776 79.434 1.00 59.05	С
ATOM	2838	NE ARG B 436	31.860 43.579 79.897 1.00 61.87	N
ATOM		CZ ARG B 436		С
ATOM			33.725 44.245 81.102 1.00 67.05	N
ATOM	2841	NH2 ARG B 436	33.260 42.010 80.867 1.00 60.90	N
ATOM	2842	N MET B 437	34.545 46.793 76.339 1.00 52.85	N
ATOM			35.013 48.137 76.084 1.00 56.56	С
ATOM		C MET B 437	34.892 48.497 74.611 1.00 54.67	С
ATOM		O MET B 437	34.292 49.542 74.301 1.00 56.44	0
ATOM		CB MET B 437	36.446 48.210 76.590 1.00 63.56	С
ATOM			36.614 49.111 77.788 1.00 74.21	С
ATOM		SD MET B 437		S
ATOM		CE MET B 437	39.287 49.222 77.049 1.00 81.39	С
ATOM	2850	N MET B 438	35.398 47.750 73.631 1.00 49.34	N
ATOM	2851	CA MET B 438	35,281 48,213 72,255 1.00 47.33	С
ATOM		C MET B 438	33.977 47.842 71.604 1.00 46.47	С
<b>ATOM</b>	2853	O MET B 438	33.850 47.985 70.374 1.00 46.26	. 0
ATOM	2854	CB MET B 438	36.371 47.632 71.348 1.00 46.13	С
<b>ATOM</b>	2855	CG MET B 438	37.616 47.220 72.115 1.00 44.79	С
<b>ATOM</b>	2856	SD MET B 438	38.883 46.590 71.100 1.00 46.76	S
<b>ATOM</b>	2857	CE MET B 438	38.508 47.061 69.426 1.00 42.55	С
<b>ATOM</b>	2858	N ASN B 439	33.010 47.339 72.341 1.00 45.12	N
<b>ATOM</b>	2859	CA ASN B 439	31.769 46.909 71.719 1.00 47.08	С
<b>ATOM</b>	2860	C ASN B 439	32.030 45.961 70.560 1.00 42.87	С
<b>ATOM</b>	2861	O ASN B 439	31.427 46.170 69.532 1.00 38.37	0
<b>ATOM</b>	2862	CB ASN B 439	30.894 48.043 71.160 1.00 54.41	С
<b>ATOM</b>	2863	CG ASN B 439	30.681 49.113 72.228 1.00 62.82	С
<b>ATOM</b>	2864	OD1 ASN B 439	30.400 48.772 73.391 1.00 68.45	0
<b>ATOM</b>	2865	ND2 ASN B 439	30.853 50.398 71.948 1.00 63.44	N
		N LEUB 440	32.836 44.915 70.767 1.00 40.15	N
<b>ATOM</b>	2867	CA LEUB 440	33.036 43.990 69.681 1.00 38.02	С
<b>ATOM</b>	2868	C LEU B 440	31.700 43.440 69.201 1.00 39.56	C
		O LEUB 440	30.812 43.082 69.978 1.00 39.57	О
		CB LEUB 440	33.945 42.860 70.083 1.00 39.03	С
ATOM	2871	CG LEUB 440	34.095 41.816 68.957 1.00 38.64	С
<b>ATOM</b>	2872	CD1 LEU B 440	34.882 42.503 67.863 1.00 40.77	С
		CD2 LEU B 440	34.781 40.613 69.567 1.00 40.57	С
		N GLN B 441	31.563 43.417 67.890 1.00 40.69	N
		CA GLN B 441	30.317 43.001 67.272 1.00 40.46	С
		C GLN B 441	30.476 41.572 66.796 1.00 41.61	С
		O GLN B 441	31.573 41.135 66.435 1.00 42.47	0
		CB GLN B 441	29.952 43.919 66.129 1.00 43.62	C
ATOM	2879	CG GLN B 441	29.793 45.380 66.436 1.00 48.63	С

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ATOM	2880 CD GLN B 441	28.646 45.620 67.426 1.00 53.79	С
ATOM	2881 OE1 GLN B 441	27.473 45.380 67.078 1.00 57.83	0
ATOM	2882 NE2 GLN B 441	28.952 46.095 68.623 1.00 50.24	N
ATOM	2883 N GLY B 442	29.358 40.858 66.803 1.00 39.15	N
ATOM	2884 CA GLY B 442	29.364 39.473 66.404 1.00 38.36	С
ATOM	2885 C GLY B 442	29.980 39.287 65.030 1.00 38.59	C
ATOM	2886 O GLY B 442	30.700 38.317 64.869 1.00 36.85	Ö
ATOM		29.673 40.200 64.107 1.00 39.06	N
ATOM		30.225 40.130 62.778 1.00 40.77	C
	2889 C GLUB 443	31.747 40.195 62.764 1.00 38.88	Č
ATOM		32.341 39.502 61.958 1.00 40.31	Ö
ATOM		29.725 41.274 61.885 1.00 43.92	Č
ATOM		28.280 40.999 61.489 1.00 49.93	č
ATOM		27.289 41.423 62.556 1.00 52.01	Č
	2894 OE1 GLU B 443	27.607 42.080 63.559 1.00 52.95	Ö
	2895 OE2 GLU B 443	26.103 41.072 62.367 1.00 56.50	Ö
_	2896 N GLUB 444	32.304 41.015 63.624 1.00 36.15	N
	2897 CA GLUB 444	33.718 41.205 63.814 1.00 34.58	Ċ
	2898 C GLUB 444	34.304 39.991 64.512 1.00 33.55	c
	2899 O GLUB 444	35.328 39.436 64.169 1.00 37.22	Ö
ATOM		33.958 42.439 64.667 1.00 34.86	Č
<b>ATOM</b>	2901 CG GLU B 444	33.459 43.740 64.094 1.00 31.42	Č
ATOM	2902 CD GLUB 444	33.675 44.906 65.062 1.00 34.07	Č
ATOM		33.134 44.858 66.203 1.00 30.06	Ö
ATOM	2904 OE2 GLU B 444	34.371 45.875 64.646 1.00 31.32	Ö
ATOM	2905 N PHE B 445	33.608 39.484 65.490 1.00 36.24	N
ATOM		34.003 38.295 66.254 1.00 35.58	C
ATOM		34.308 37.128 65.357 1.00 35.27	C
ATOM	2908 O PHE B 445	35.313 36.412 65.412 1.00 40.19	Ö
ATOM	2909 CB PHE B 445		C
ATOM	2910 CG PHE B 445		Č
ATOM	2911 CD1 PHE B 445	34.034 36.211 68.566 1.00 25.60	С
	2912 CD2 PHE B 445		Č
	2913 CE1 PHE B 445		C
ATOM	2914 CE2 PHE B 445		C
	2915 CZ PHE B 445	33.127 33.951 68.828 1.00 28.70	C
ATOM	2916 N VAL B 446	33.340 36.823 64.553 1.00 34.10	N
<b>ATOM</b>	2917 CA VAL B 446	33,325 35.647 63.645 1.00 34.65	С
ATOM	2918 C VAL B 446	34.441 35.755 62.659 1.00 35.98	С
<b>ATOM</b>	2919 O VAL B 446	35.089 34.817 62.161 1.00 35.51	0
ATOM	2920 CB VAL B 446	31.855 35.683 63.194 1.00 34.90	C
<b>ATOM</b>	2921 CG1 VAL B 446	31.527 35.886 61.769 1.00 32.60	С
<b>ATOM</b>	2922 CG2 VAL B 446	31.123 34.554 63.911 1.00 32.13	С
	2923 N CYS B 447	34.751 37.011 62.335 1.00 36.12	N
	2924 CA CYS B 447	35.830 37.341 61.416 1.00 36.00	C
	2925 C CYS B 447	37.163 37.010 62.071 1.00 37.62	C
	2926 O CYS B 447	38.056 36.366 61.498 1.00 37.88	Ō
	2927 CB CYS B 447	35.638 38.810 61.119 1.00 35.26	C
	2928 SG CYS B 447	34.873 39.112 59.520 1.00 36.98	S
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43.622 33.306 61.687 1.00 34.48 0 ATOM 2955 O ILE B 451 C ATOM 2956 CB ILE B 451 41.877 36.109 61.474 1.00 26.02 41.408 37.037 60.331 1.00 23.22 ATOM 2957 CG1 ILE B 451 ATOM 2958 CG2 ILE B 451 43.361 36.401 61.672 1.00 29.64 C 41.256 38.461 60.801 1.00 18.98 ATOM 2959 CD1 ILE B 451 ATOM 2960 N ILE B 452 42.099 33.533 63.249 1.00 30.12 N 42.843 32.711 64.175 1.00 29.93 C ATOM 2961 CA ILE B 452 ATOM 2962 C ILE B 452 43.056 31.337 63.559 1.00 31.42 ATOM 2963 O ILE B 452 44.195 30.815 63.582 1.00 34.08 0 ATOM 2964 CB ILE B 452 42.144 32.606 65.550 1.00 28.86 ATOM 2965 CG1 ILE B 452 42.345 33.913 66.330 1.00 26.71 ATOM 2966 CG2 ILE B 452 42.556 31.429 66.392 1.00 22.07 C ATOM 2967 CD1 ILE B 452 41.556 33.907 67.645 1.00 25.52 C ATOM 2968 N LEUB 453 42.019 30.719 63.057 1.00 30.00 N ATOM 2969 CA LEUB 453 42.178 29.363 62.504 1.00 33.56 C ATOM 2970 C LEU B 453 43,230 29,315 61,378 1.00 34.89 C ATOM 2971 O LEUB 453 44.116 28.440 61.327 1.00 31.76 0 ATOM 2972 CB LEUB 453 40.849 28.894 61.906 1.00 31.42 ATOM 2973 CG LEU B 453 40.852 27.667 61.019 1.00 28.92 ATOM 2974 CD1 LEU B 453 41.063 26.366 61.798 1.00 24.08 C ATOM 2975 CD2 LEU B 453 39.503 27.591 60.278 1.00 30.58 C ATOM 2976 N LEUB 454 43.077 30.262 60.454 1.00 34.10 N ATOM 2977 CA LEUB 454 43.928 30.393 59.312 1.00 35.40

ATOM 3027 N TYR B 459 52.686 28.951 59.520 1.00101.08 N C ATOM 3028 CA TYR B 459 54.118 28.829 59.478 1.00105.58 ATOM 3029 C TYR B 459 54.628 27.383 59.505 1.00106.66 C ATOM 3030 O TYR B 459 55.476 27.053 60.360 1.00106.92 0 54.759 29.538 60.691 1.00108.78 ATOM 3031 CB TYR B 459 ATOM 3032 CG TYR B 459 54.932 31.015 60.441 1.00112.75 54.140 31.670 59.507 1.00114.02 C ATOM 3033 CD1 TYR B 459 C ATOM 3034 CD2 TYR B 459 55.888 31.764 61.118 1.00113.67 C ATOM 3035 CE1 TYR B 459 54.269 33.009 59.243 1.00114.56 ATOM 3036 CE2 TYR B 459 56.030 33.115 60.860 1.00114.48 C ATOM 3037 CZ TYR B 459 55.220 33.728 59.937 1.00114.74 C ATOM 3038 OH TYR B 459 55.309 35.074 59.662 1.00115.64 0 ATOM 3039 N LEUB 469 53.455 26.042 47.196 1.00114.47 N ATOM 3040 CA LEUB 469 53.703 27.415 47.649 1.00113.63 C ATOM 3041 C LEUB 469 52.595 28.339 47.164 1.00111.18 C ATOM 3042 O LEUB 469 52.452 29.481 47.572 1.00110.61 0 55.056 27.927 47.145 1.00114.74 C ATOM 3043 CB LEU B 469 51.735, 27.749 46.323 1.00108.99 ATOM 3047 N GLUB 470 ATOM 3048 CA GLUB 470 50.552 28.514 45.891 1.00107.74 C 49.492 28.303 46.983 1.00106.21 ATOM 3049 C GLUB 470 C ATOM 3050 O GLUB 470 48.424 28.886 46.982 1.00106.32 0 ATOM 3051 CB GLUB 470 50.083 28.142 44.510 1.00107.28 C ATOM 3056 N GLUB 471 49.832 27.431 47.915 1.00103.94 N 49.046 27.060 49.063 1.00102.02 C ATOM 3057 CA GLU B 471 49.190 28.135 50.131 1.00 99.15 ATOM 3058 C GLUB 471 ATOM 3059 O GLU B 471 48.228 28.784 50.542 1.00100.18 0 ATOM 3060 CB GLUB 471 49.505 25.692 49.591 1.00102.87 C ATOM 3065 N LYSB 472 50.438 28.412 50.518 1.00 95.05 N 50.694 29.474 51.488 1.00 90.18 C ATOM 3066 CA LYS B 472 ATOM 3067 C LYS B 472 49.906 30.708 51.018 1.00 85.61 C ATOM 3068 O LYS B 472 49.154 31.313 51.764 1.00 85.79 0 C 52.164 29.863 51.584 1.00 90.78 ATOM 3069 CB LYS B 472 ATOM 3074 N ASP B 473 50.106 30.995 49.743 1.00 79.96 N ATOM 3075 CA ASP B 473 49.463 32.091 49.096 1.00 76.18 C ATOM 3076 C ASP B 473 47.971 32.104 49.117 1.00 70.30 C ATOM 3077 O ASP B 473 47.343 33.158 49.225 1.00 68.00 0 ATOM 3078 CB ASP B 473 50.058 32.230 47.670 1.00 79.82 C ATOM 3079 CG ASP B 473 50.812 33.579 47.744 1.00 85.00 51.707 33.695 48.625 1.00 87.11 ATOM 3080 OD1 ASP B 473 0 ATOM 3081 OD2 ASP B 473 50.338 34.479 47.015 1.00 86.01 0 47.315 30.960 49.042 1.00 67.17 N ATOM 3082 N HISB 474 ATOM 3083 CA HIS B 474 45.859 30.919 49.049 1.00 64.04 C C ATOM 3084 C HISB 474 45.313 31.500 50.359 1.00 59.13 44.512 32.421 50.406 1.00 54.26 0 ATOM 3085 O HIS B 474 ATOM 3086 CB HIS B 474 45.373 29.472 48.872 1.00 65.44 C ATOM 3087 CG HIS B 474 43.869 29.373 48.910 1.00 66.08 C 43.042 30.096 48.057 1.00 64.73 N ATOM 3088 ND1 HIS B 474 C ATOM 3089 CD2 HIS B 474 43.085 28.640 49.749 1.00 63.86 41.788 29.791 48.371 1.00 65.57 C ATOM 3090 CE1 HIS B 474

ATOM			41.798 28.914 49.383 1.00 65.82	N
ATOM		N ILE B 475	45.796 30.880 51.428 1.00 54.85	N
ATOM			45.486 31.241 52.789 1.00 52.82	С
ATOM		C ILE B 475	45.684 32.719 52.997 1.00 52.67	C
ATOM		O ILE B 475	44.795 33.382 53.573 1.00 52.33	0
ATOM			46.369 30.407 53.743 1.00 53.77	C
			45.613 29.092 54.003 1.00 55.72	C
ATOM			46.702 31.124 55.023 1.00 50.98	C
ATOM		CD1 ILE B 475	45.981 28.459 55.332 1.00 57.41	С
<b>ATOM</b>		N HIS B 476	46.807 33.259 52.541 1.00 51.23	N
			47.093 34.668 52.664 1.00 56.36	С
		C HIS B 476	46.068 35.544 51.960 1.00 57.23	С
		O HIS B 476	45.771 36.671 52.356 1.00 59.56	0
			48.489 34.972 52.119 1.00 62.85	C
			49.496 34.811 53.217 1.00 73.21	С
<b>ATOM</b>	3106	ND1 HIS B 476	50.291 33.686 53.347 1.00 76.61	N
		CD2 HIS B 476	49.789 35.602 54.290 1.00 75.57	С
			51.057 33.808 54.416 1.00 76.91	С
<b>ATOM</b>	3109	NE2 HIS B 476	50.750 34.949 55.019 1.00 76.75	N
<b>ATOM</b>	3110	N ARG B 477		N
		<b>CA ARG B 477</b>	44.499 35.781 50.123 1.00 55.00	С
		C ARG B 477		C
<b>ATOM</b>	3113	O ARG B 477		0
		CB ARG B 477		С
ATOM	3115	CG ARG B 477	45.762 35.404 47.984 1.00 64.22	С
ATOM	3116	CD ARG B 477		С
ATOM	3117	NE ARG B 477		N
ATOM	3121	N VAL B 478		N
		CA VAL B 478	41.689 34.417 52.255 1.00 45.48	С
		C VAL B 478		С
			40.824 36.191 53.631 1.00 40.18	0
ATOM	3125	CB VAL B 478		C
ATOM	3126	CG1 VAL B 478	40.250 32.944 53.660 1.00 42.28	С
		CG2 VAL B 478	41.454 31.965 51.700 1.00 42.27	С
		N LEUB 479	42.928 35.425 54.060 1.00 42.57	N
		CA LEU B 479		С
		C LEU B 479	43.018 37.825 54.643 1.00 38.95	C
		O LEU B 479	42.407 38.618 55.374 1.00 44.89	0
		CB LEU B 479	44.598 36.247 55.697 1.00 38.43	C
		CG LEU B 479		C
		CD1 LEU B 479		C
		CD2 LEU B 479		C
		N ASP B 480	43.481 38.218 53.498 1.00 37.41	N
		CA ASP B 480	43.276 39.561 52.966 1.00 39.12	С
		C ASP B 480	41.776 39.859 52.822 1.00 39.72	C
		O ASP B 480	41.244 40.935 53.171 1.00 37.31	0
		CB ASP B 480	43.919 39.686 51.598 1.00 40.28	C
		CG ASP B 480		C
ATOM	3142	OD1 ASP B 480	46.014 40.191 52.637 1.00 45.55	0

<b>ATOM</b>	3143	OD2 ASP B 480	45.934 40.346 50.526 1.00 50.28	0
<b>ATOM</b>	3144	N LYS B 481	41.060 38.846 52.311 1.00 37.19	N
<b>ATOM</b>	3145	CA LYS B 481	39.626 39.005 52.153 1.00 39.36	С
<b>ATOM</b>	3146	C LYSB 481	38.942 39.231 53.490 1.00 37.52	С
<b>ATOM</b>	3147	O LYS B 481	38.052 40.083 53.640 1.00 33.55	Ο
			39.076 37.807 51.405 1.00 44.24	С
			37.767 38.132 50.733 1.00 51.43	С
<b>ATOM</b>	3150	CD LYS B 481	37.705 37.779 49.253 1.00 54.23	С
			36.592 38.657 48.653 1.00 55.57	С
<b>ATOM</b>	3152	NZ LYS B 481	37.061 39.411 47.470 1.00 60.01	N
<b>ATOM</b>	3153	N ILE B 482	39.455 38.536 54.537 1.00 35.79	N
<b>ATOM</b>	3154	CA ILE B 482	38.872 38.765 55.867 1.00 33.69	С
<b>ATOM</b>	3155	C ILE B 482	39.141 40.146 56.389 1.00 34.23	С
<b>ATOM</b>	3156	O ILE B 482	38.239 40.803 56.970 1.00 35.10	Ο
<b>ATOM</b>	3157	CB ILE B 482	39.092 37.644 56.819 1.00 31.16	С
<b>ATOM</b>	3158	CG1 ILE B 482	38.922 36.299 56.067 1.00 24.05	С
<b>ATOM</b>	3159	CG2 ILE B 482	38.101 37.675 57.989 1.00 31.64	С
<b>ATOM</b>	3160	CD1 ILE B 482	38.933 35.211 57.089 1.00 25.98	С
<b>ATOM</b>	3161	N THR B 483	40.332 40.657 56.099 1.00 33.25	N
<b>ATOM</b>	3162	CA THR B 483	40.643 42.033 56.499 1.00 33.50	С
<b>ATOM</b>	3163	C THR B 483	39.644 42.958 55.811 1.00 35.50	С
<b>ATOM</b>	3164	O THR B 483	39.015 43.787 56.417 1.00 36.34	0
<b>ATOM</b>	3165	CB THR B 483	42.066 42.428 56.055 1.00 32.03	С
<b>ATOM</b>	3166	OG1 THR B 483	43.012 41.542 56.714 1.00 31.73	О
			42.368 43.871 56.435 1.00 23.76	С
		N ASP B 484		N
<b>ATOM</b>	3169	CA ASP B 484	38.526 43.498 53.678 1.00 39.14	С
<b>ATOM</b>	3170	C ASP B 484	37.150 43.443 54.309 1.00 38.08	С
		O ASP B 484		О
			38.415 42.904 52.293 1.00 42.39	C
			39.624 43.139 51.453 1.00 45.80	C
			40.287 44.189 51.613 1.00 51.95	0
		OD2 ASP B 484	39.958 42.283 50.636 1.00 48.98	0
-		N THR B 485	36.702 42.236 54.635 1.00 36.36	N
		CA THR B 485		С
ATOM			35.396 42.874 56.589 1.00 39.62	C
		O THR B 485	34.469 43.641 56.847 1.00 42.09	0
		CB THR B 485	35.092 40.639 55.602 1.00 35.78	C
		OG1 THR B 485		0
		CG2 THR B 485		C
		N LEUB 486	36.455 42.687 57.410 1.00 40.70	N
		CA LEUB 486	36.524 43.442 58.661 1.00 39.17	С
		C LEUB 486	36.357 44.937 58.426 1.00 36.46	C
		O LEUB 486		0
		CB LEUB 486	37.819 43.240 59.397 1.00 37.63	C
		CG LEUB 486	37.839 42.538 60.735 1.00 39.49	C
		CD1 LEU B 486		C
		CD2 LEU B 486		C
ATOM	3191	N ILE B 487	37.092 45.487 57.475 1.00 37.80	N

ATOM			36.971 46.933 57.230 1.00 41.68	С
<b>ATOM</b>			35.587 47.346 56.741 1.00 40.87	C
<b>ATOM</b>	3194	O ILE B 487	35.023 48.354 57.126 1.00 37.88	0
ATOM	3195	CB ILE B 487	38.025 47.395 56.224 1.00 40.44	С
<b>ATOM</b>	3196	CG1 ILE B 487	39.414 47.123 56.770 1.00 39.53	С
<b>ATOM</b>	3197	CG2 ILE B 487	37.795 48.871 55.903 1.00 39.33	С
<b>ATOM</b>	3198	CD1 ILE B 487		С
ATOM	3199	N HISB 488	35.038 46.545 55.855 1.00 45.86	N
<b>ATOM</b>		CA HIS B 488	33.689 46.702 55.338 1.00 47.90	С
ATOM	3201	C HIS B 488	32.692 46.897 56.470 1.00 45.88	С
<b>ATOM</b>	3202			0
ATOM			33.346 45.498 54.470 1.00 50.31	С
ATOM		CG HIS B 488	31.959 45.674 53.895 1.00 56.89	С
ATOM		ND1 HIS B 488	30.859 44.934 54.302 1.00 57.87	N
		CD2 HIS B 488	31.534 46.527 52.925 1.00 56.23	С
		CE1 HIS B 488	29.809 45.323 53.611 1.00 58.24	C
ATOM		NE2 HIS B 488	30.211 46.273 52.783 1.00 58.77	N
ATOM		N LEUB 489	32.631 45.959 57.417 1.00 43.00	N
ATOM		CA LEU B 489		C
		C LEUB 489		С
		O LEUB 489	31.040 48.016 59.786 1.00 39.75	0
		CB LEU B 489	31.976 44.978 59.566 1.00 34.08	C
		CG LEU B 489		C
		CD1 LEU B 489		C
		CD2 LEU B 489		C
ATOM		N MET B 490	33.240 47.814 59.347 1.00 43.79	N
ATOM		CA MET B 490	33.547 49.059 60.077 1.00 46.64	C
ATOM	3219		33.001 50.287 59.363 1.00 44.69	Ö
ATOM		O MET B 490	32.379 51.103 60.020 1.00 39.83 35.010 49.207 60.413 1.00 45.72	C
ATOM	3221		35.437 48.611 61.751 1.00 44.92	C
ATOM	3222			S
		SD MET B 490 CE MET B 490	37.054 46.523 62.575 1.00 44.78	C
ATOM		N ALAB 491	33.208 50.332 58.056 1.00 48.14	N.
		CA ALA B 491	32.766 51.454 57.213 1.00 49.71	C
		C ALA B 491	31.248 51.491 57.282 1.00 55.03	c
		O ALA B 491	30.614 52.476 57.607 1.00 56.54	ŏ
		CB ALA B 491	33.213 51.273 55.791 1.00 42.64	C
		N LYS B 492	30.681 50.309 57.031 1.00 59.07	N
		CA LYS B 492	29.233 50.124 57.088 1.00 61.88	C
		C LYS B 492	28.694 50.716 58.374 1.00 61.14	C
		O LYS B 492	27,738 51,490 58,326 1.00 65.25	0
		CB LYS B 492	28.912 48.648 56.973 1.00 65.85	С
		CG LYS B 492	27.487 48.224 56.873 1.00 70.73	С
		CD LYS B 492	27.335 46.970 56.007 1.00 75.73	С
		CE LYS B 492	25.939 47.010 55.356 1.00 79.99	С
		NZ LYS B 492	25,382 45.631 55.150 1.00 83.64	N
		N ALA B 493	29.300 50.465 59.505 1.00 59.06	N
		CA ALA B 493	28.979 50.984 60.803 1.00 58.83	С

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ATOM	3241	C ALA B 493		С
		O ALA B 493		0
			29.902 50.311 61.828 1.00 58.13	С
		N GLY B 494		N
		CA GLY B 494		С
<b>ATOM</b>	3246	C GLY B 494		С
<b>ATOM</b>			31.413 56.184 60.897 1.00 66.15	Ο
		N LEU B 495		N
			33.613 54.731 61.339 1.00 55.79	С
		C LEU B 495		С
		O LEU B 495		Ο
			34.497 53.673 61.886 1.00 52.94	С
			34.054 52.508 62.694 1.00 50.03	С
			35.176 52.086 63.635 1.00 50.56	С
<b>ATOM</b>	3255	CD2 LEU B 495	32.772 52.721 63.431 1.00 48.72	С
		N THR B 496		N
		CA THR B 496		С
<b>ATOM</b>	3258	C THR B 496	37.014 56.202 59.035 1.00 55.30	С
<b>ATOM</b>				0
		CB THR B 496		С
		OG1 THR B 496		О
			35.368 59.344 60.587 1.00 56.74	С
			37.732 56.636 58.027 1.00 56.81	N
			38.809 55.838 57.461 1.00 58.93	C
		C LEU B 497		C
ATOM		O LEU B 497		Ο.
ATOM			39.406 56.537 56.248 1.00 57.10	C
			38.864 55.921 54.946 1.00 60.97	C
			38.737 56.909 53.812 1.00 61.29	C
			39.749 54.735 54.590 1.00 61.42	C
			40.116 56.642 59.298 1.00 60.04	N
		CA GLN B 498		С
ATOM		C GLN B 498	40.655 55.619 61.429 1.00 56.58	C
		O GLN B 498	41.383 54.779 61.906 1.00 54.84	0
		CB GLN B 498	41.322 57.959 60.954 1.00 59.96	C
		CG GLN B 498	42.003 57.852 62.316 1.00 64.82	C
		CD GLN B 498	42.807 59.111 62.587 1.00 66.88	C
<del>-</del> -		OE1 GLN B 498	42.325 59.914 63.377 1.00 70.04	0
		NE2 GLN B 498	43.951 59.235 61.948 1.00 68.14	N
		N GLN B 499	39.387 55.786 61.796 1.00 56.24	N
		CA GLN B 499	38.822 54.914 62.829 1.00 56.35	C
		C GLN B 499	38.856 53.453 62.393 1.00 56.05	С
		O GLN B 499	39.074 52.610 63.264 1.00 57.20	0
		CB GLN B 499	37.424 55.348 63.149 1.00 55.66	C
		CG GLN B 499	37.327 56.721 63.773 1.00 56.83	C
		CD GLN B 499	35.871 56.986 64.130 1.00 58.69	C
		OE1 GLN B 499	35.006 56.866 63.274 1.00 58.39	0 N
		NE2 GLN B 499	35.642 57.324 65.385 1.00 61.19	N
АТОМ	3289	N GLN B 500	38.623 53.155 61.132 1.00 52.26	N

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ATOM			38.721 51.832 60.580 1.00 48.06	
<b>ATOM</b>	3291	C GLN B 500		С
<b>ATOM</b>	3292	O GLN B 500	40.155 50.095 61.389 1.00 51.62	0
<b>ATOM</b>	3293	CB GLN B 500	38.513 51.894 59.041 1.00 <b>45.29</b>	C
<b>ATOM</b>	3294	CG GLN B 500	37.067 51.860 58.683 1.00 45.42	С
<b>ATOM</b>	3295	CD GLN B 500	36.618 52.564 57.441 1.00 45.44	С
<b>ATOM</b>	3296	OE1 GLN B 500	37.103 52.308 56.351 1.00 46.78	0
<b>ATOM</b>	3297	NE2 GLN B 500	35.648 53.468 57.589 1.00 44.47	N
<b>ATOM</b>	3298	N AHIS B 501	41.170 51.777 60.317 0.50 46.65	N
<b>ATOM</b>	3299	N BHIS B 501	41.099 51.854 60.328 0.50 47.93	N
<b>ATOM</b>	3300	CA AHIS B 501	42.463 51.100 60.524 0.50 43.55	С
<b>ATOM</b>	3301	CA BHIS B 501	42.477 51.385 60.430 0.50 46.45	С
<b>ATOM</b>	3302	C AHIS B 501	42.770 50.998 62.015 0.50 44.08	С
<b>ATOM</b>	3303	C BHIS B 501	42.918 51.257 61.881 0.50 45.96	С
<b>ATOM</b>	3304	O AHIS B 501	43.503 50.096 62.434 0.50 46.22	0
<b>ATOM</b>	3305	O BHIS B 501	43.586 50.264 62.211 0.50 47.87	0
<b>ATOM</b>	3306	CB AHIS B 501	43.619 51.724 59.805 0.50 41.42	С
ATOM	3307	CB BHIS B 501	43.367 52.356 59.651 0.50 47.09	С
<b>ATOM</b>	3308	CG AHIS B 501	43.981 53.129 60.147 0.50 40.96	С
<b>ATOM</b>	3309	CG BHIS B 501	43.020 52,436 58,188 0,50 48,40	С
<b>ATOM</b>	3310	ND1AHIS B 501	44.259 54.067 59.171 0.50 41.42	N
ATOM	3311	ND1BHIS B 501	42.555 51.328 57.498 0.50 48.78	N
			44.121 53.774 61.328 0.50 40.78	С
<b>ATOM</b>	3313	CD2BHIS B 501	43.114 53.436 57.281 0.50 46.35	C
<b>ATOM</b>	3314	CE1AHIS B 501	44.534 55.223 59.764 0.50 43.40	С
<b>ATOM</b>	3315	CE1BHIS B 501	42.368 51.660 56.234 0.50 48.60	С
<b>ATOM</b>	3316	NE2AHIS B 501	44.438 55.078 61.079 0.50 40.95	N
<b>ATOM</b>	3317	NE2BHIS B 501	42.705 52.928 56.081 0.50 46.13	N
<b>ATOM</b>	3318	N GLN B 502	42.228 51.930 62.808 1.00 42.77	N
<b>ATOM</b>	3319	CA GLN B 502	42.557 51.941 64.220 1.00 40.75	С
<b>ATOM</b>	3320	C GLN B 502	41.919 50.773 64.947 1.00 39.12	С
<b>ATOM</b>	3321	O GLN B 502	42.647 50.028 65.601 1.00 36.67	0
<b>ATOM</b>	3322	CB GLN B 502	42.252 53.228 64.935 1.00 38.57	С
<b>ATOM</b>	3323	CG GLN B 502	43.059 54.353 64.298 1.00 40.97	С
<b>ATOM</b>	3324	CD GLN B 502	43.087 55.565 65.193 1.00 42.76	С
<b>ATOM</b>	3325	OE1 GLN B 502	44.039 56.323 65.007 1.00 49.28	0
<b>ATOM</b>	3326	<b>NE2 GLN B 502</b>	42.164 55.761 66.094 1.00 42.12	N
<b>ATOM</b>	3327	N ARG B 503	40.630 50.621 64.649 1.00 39.47	N
<b>ATOM</b>	3328	CA ARG B 503	39.864 49.519 65.188 1.00 36.78	С
<b>ATOM</b>	3329	C ARG B 503	40.427 48.201 64.642 1.00 34.42	С
<b>ATOM</b>	3330	O ARG B 503	40.677 47.297 65.427 1.00 34.41	0
<b>ATOM</b>	3331	CB ARG B 503	38.410 49.557 64.829 1.00 36.81	С
<b>ATOM</b>	3332	CG ARG B 503	37.638 48.456 65.653 1.00 35.98	С
<b>ATOM</b>	3333	CD ARG B 503	36.179 48.843 65.506 1.00 35.57	С
<b>ATOM</b>	3334	NE ARG B 503		N
<b>ATOM</b>	3335	CZ ARG B 503	34.997 47.930 67.391 1.00 42.50	С
<b>ATOM</b>	3336	NH1 ARG B 503	35.680 48.835 68.083 1.00 44.65	N
ATOM	3337	NH2 ARG B 503	34.169 47.071 67.944 1.00 43.19	N
<b>ATOM</b>	3338	N LEUB 504	40.726 48.172 63.368 1.00 32.25	N

ATOM 3339 CA LEU B 504 41,292 46,936 62,823 1,00 33.65 C C 42.525 46.549 63.601 1.00 36.37 ATOM 3340 C LEUB 504 0 42.718 45.361 63.937 1.00 38.64 ATOM 3341 O LEUB 504 41.649 47.125 61.351 1.00 32.77 C ATOM 3342 CB LEU B 504 42.329 45.917 60.688 1.00 28.02 ATOM 3343 CG LEU B 504 ATOM 3344 CD1 LEU B 504 41.351 44.779 60.549 1.00 20.13 42,931 46,378 59,373 1,00 23,43 C ATOM 3345 CD2 LEU B 504 43.388 47.540 63.857 1.00 37.99 N ATOM 3346 N ALA B 505 44.651 47.278 64.606 1.00 31.73 C ATOM 3347 CA ALA B 505 ATOM 3348 C ALA B 505 44.359 46.883 66.023 1.00 29.70 C ATOM 3349 O ALA B 505 44.932 45.965 66.578 1.00 26.36 0 C 45.503 48.523 64.577 1.00 32.14 ATOM 3350 CB ALA B 505 43.415 47.597 66.669 1.00 33.66 ATOM 3351 N GLN B 506 N C ATOM 3352 CA GLN B 506 43.046 47.218 68.038 1.00 35.30 ATOM 3353 C GLN B 506 42.616 45.755 68.063 1.00 36.27 C 43.246 45.000 68.820 1.00 39.25 ATOM 3354 O GLN B 506 0 ATOM 3355 CB GLN B 506 41.990 48.086 68.669 1.00 35.30 C ATOM 3356 CG GLN B 506 42.394 49.533 68.813 1.00 39.85 41.214 50.474 68.812 1.00 45.28 ATOM 3357 CD GLN B 506 40.128 50.163 69.315 1.00 49.60 ATOM 3358 OE1 GLN B 506 ATOM 3359 NE2 GLN B 506 41.392 51.660 68.253 1.00 49.18 N 41.690 45.322 67.198 1.00 32.30 ATOM 3360 N LEUB 507 N 41.346 43.911 67.223 1.00 30.88 ATOM 3361 CA LEUB 507 C 42.491 42.993 66.935 1.00 29.84 ATOM 3362 C LEUB 507 C 42.616 41.987 67.596 1.00 31.13 O ATOM 3363 O LEUB 507 ATOM 3364 CB LEUB 507 40.259 43.609 66.138 1.00 32.27 ATOM 3365 CG LEUB 507 39.091 44.575 66.311 1.00 33.70 38.048 44.471 65.247 1.00 34.24 ATOM 3366 CD1 LEU B 507 C 38.559 44.294 67.697 1.00 35.31 ATOM 3367 CD2 LEU B 507 43.350 43.211 65.930 1.00 31.10 N ATOM 3368 N LEUB 508 ATOM 3369 CA LEU B 508 44.400 42.227 65.712 1.00 30.54 C C ATOM 3370 C LEUB 508 45.435 42.214 66.800 1.00 30.57 ATOM 3371 O LEUB 508 45.928 41.097 66.978 1.00 33.14 0 45.035 42.228 64.339 1.00 29.19 ATOM 3372 CB LEU B 508 ATOM 3373 CG LEU B 508 43.984 42.309 63.217 1.00 30.62 44.677 42.905 62.014 1.00 31.84 ATOM 3374 CD1 LEU B 508 C ATOM 3375 CD2 LEU B 508 43.354 40.958 63.003 1.00 26.58 ATOM 3376 N LEUB 509 45.638 43.235 67.613 1.00 28.82 N 46.620 43.082 68.682 1.00 27.22 C ATOM 3377 CA LEUB 509 C ATOM 3378 C LEUB 509 46.035 42.165 69.719 1.00 30.73 ATOM 3379 O LEUB 509 46.837 41.469 70.369 1.00 32.94 0 ATOM 3380 CB LEU B 509 47.031 44.405 69.286 1.00 29.04 47.727 45.304 68.242 1.00 28.79 ATOM 3381 CG LEU B 509 ATOM 3382 CD1 LEU B 509 C 48.237 46.507 68.932 1.00 35.11 48.860 44.511 67.641 1.00 28.05 C ATOM 3383 CD2 LEU B 509 ATOM 3384 N ILE B 510 44.709 42.129 69.838 1.00 30.11 N ATOM 3385 CA ILE B 510 44.065 41.203 70.781 1.00 30.61 C 44.378 39.793 70.326 1.00 30.81 C ATOM 3386 C ILE B 510 44.466 38.844 71.147 1.00 32.18 0 ATOM 3387 O ILE B 510

wo 9	98/56812		PCT/GB98/01708
	,	99/371	
		42.576 41.539 70.920 1.00 35.88	С
		42.321 42.740 71.838 1.00 39.34	C
		41.722 40.376 71.437 1.00 34.95	
	3391 CD1 ILE B 510		
	3392 N LEUB 511		N
		45.034 38.192 68.643 1.00 28.74	С
		46.368 37.876 69.273 1.00 30.01	C
		46.433 36.716 69.732 1.00 35.16	0
		45.001 37.896 67.156 1.00 26.69	С
		43.616 38.137 66.479 1.00 26.06	C
		43.726 37.691 65.044 1.00 16.51	C
	3399 CD2 LEU B 511		C
	3400 N SER B 512	47.371 38.676 69.552 1.00 29.76 48.520 38.200 70.312 1.00 31.98	N
		48.320 38.200 70.312 1.00 31.98	C C
		48.933 36.829 72.224 1.00 30.49	0
		49.652 39.244 70.422 1.00 35.44	C
		49.319 40.233 69.447 1.00 46.47	Ö
	3406 N HIS B 513		N
		47.015 38.093 73.790 1.00 32.67	Ċ
	3408 C HIS B 513		C
	3409 O HIS B 513	· ·	Ō
		46.062 39.120 74.347 1.00 34.61	С
ATOM	3411 CG HIS B 513	46.660 40.486 74.389 1.00 37.60	С
ATOM	3412 ND1 HIS B 513	47.777 40.752 75.169 1.00 41.78	N
ATOM	3413 CD2 HIS B 513	46.307 41.641 73.838 1.00 42.38	С
ATOM	3414 CE1 HIS B 513	48.086 42.014 75.057 1.00 44.76	
		47.216 42.599 74.230 1.00 47.20	N
		45.397 36.604 72.843 1.00 34.02	N
		44.770 35.276 72.708 1.00 33.15	C
		45.820 34.235 72.495 1.00 32.37	C
	3419 O ILE B 514	45.878 33.229 73.224 1.00 34.97	0
	3420 CB ILE B 514	43.635 35.391 71.710 1.00 32.90	C
	3421 CG1 ILE B 514	42.445 36.115 72.387 1.00 29.27	C
	3422 CG2 ILE B 514	43.169 34.033 71.236 1.00 34.89	C
	3423 CD1 ILE B 514	41.575 36.805 71.391 1.00 32.54	C .
	3424 N ARG B 515 3425 CA ARG B 515	46.768 34.357 71.566 1.00 32.82 47.815 33.347 71.392 1.00 30.13	N C
	3426 C ARG B 515	48.528 33.144 72.713 1.00 30.92	c
	3427 O ARG B 515	48.779 32.095 73.242 1.00 32.38	0
	3428 CB ARGB 515	48.779 32.093 73.242 1.00 32.38	C
	3429 CG ARG B 515	50.056 33.038 70.203 1.00 32.12	C
	3430 CD ARG B 515	49.706 31.820 69.408 1.00 35.87	Č
	3431 NE ARG B 515	50.513 31.578 68.211 1.00 39.98	N
	3432 CZ ARG B 515	50.021 31.993 67.036 1.00 43.57	C
	3433 NH1 ARG B 515		N
	3434 NH2 ARG B 515		N
	3435 N HIS B 516	48.861 34.252 73.371 1.00 33.83	N
ATOM	3436 CA HIS B 516	49.522 34.215 74.650 1.00 31.88	С
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ATOM	3437 C HIS B 516	48.727 33.345 75.581 1.00 31.82	C
ATOM		49.258 32.370 76.082 1.00 35.15	0
ATOM		49.768 35.645 75.138 1.00 33.80	C
ATOM		50.718 35.637 76.327 1.00 39.24	С
ATOM	3441 ND1 HIS B 516	52.021 35.172 76.282 1.00 37.28	N
ATOM		50.503 36.045 77.616 1.00 37.42	С
<b>ATOM</b>	3443 CE1 HIS B 516	52.531 35.272 77.481 1.00 35.00	С
<b>ATOM</b>	3444 NE2 HIS B 516	51.655 35.796 78.288 1.00 35.03	N
<b>ATOM</b>	3445 N MET B 517	47.455 33.591 75.850 1.00 31.17	N
<b>ATOM</b>	3446 CA MET B 517	46.668 32.737 76.744 1.00 28.29	C
<b>ATOM</b>	3447 C MET B 517	46.685 31.324 76.296 1.00 30.07	С
<b>ATOM</b>	3448 O MET B 517	46.927 30.420 77.095 1.00 30.86	0
<b>ATOM</b>	3449 CB MET B 517	45.242 33.276 76.730 1.00 32.23	С
<b>ATOM</b>	3450 CG MET B 517	45.217 34.646 77.408 1.00 31.26	С
<b>ATOM</b>	3451 SD MET B 517	43.573 35.270 77.608 1.00 37.21	S
<b>ATOM</b>	3452 CE MET B 517	43.181 35.765 75.937 1.00 28.84	С
<b>ATOM</b>	3453 N SER B 518	46.527 31.089 74.977 1.00 30.90	N
<b>ATOM</b>	3454 CA SER B 518	46.600 29.676 74.543 1.00 31.77	С
<b>ATOM</b>	3455 C SER B 518	47.939 29.094 74.903 1.00 31.54	С
ATOM	3456 O SER B 518	48.073 28.045 75.505 1.00 33.26	0
ATOM	3457 CB SER B 518	46.369 29.547 73.033 1.00 32.22	С
<b>ATOM</b>	3458 OG SER B 518	46.480 28.189 72.666 1.00 29.39	0
<b>ATOM</b>	3459 N ASN B 519	49.028 29.748 74.511 1.00 32.87	N
<b>ATOM</b>	3460 CA ASN B 519	50.339 29.190 74.896 1.00 35.57	C
<b>ATOM</b>	3461 C ASN B 519	50.367 28.942 76.372 1.00 39.13	С
ATOM	3462 O ASN B 519	50.678 27.857 76.863 1.00 41.01	Ο
ATOM	3463 CB ASN B 519	51.430 30.134 74.396 1.00 33.23	С
<b>ATOM</b>	3464 CG ASN B 519	51.575 29.969 72.886 1.00 35.23	С
<b>ATOM</b>	3465 OD1 ASN B 519	51.665 30.870 72.076 1.00 38.85	0
<b>ATOM</b>	3466 ND2 ASN B 519	51.590 28.729 72.404 1.00 37.47	N
<b>ATOM</b>	3467 N LYS B 520	49.985 29.912 77.222 1.00 41.55	N
<b>ATOM</b>	3468 CA LYS B 520	50.060 29.627 78.653 1.00 44.34	С
<b>ATOM</b>	3469 C LYS B 520	49.141 28.477 79.024 1.00 46.36	С
<b>ATOM</b>	3470 O LYS B 520	49.528 27.609 79.802 1.00 47.82	Ο
<b>ATOM</b>	3471 CB LYS B 520	49.763 30.907 79.435 1.00 47.11	C
<b>ATOM</b>	3472 CG LYS B 520	50.795 31.979 79.139 1.00 55.94	С
<b>ATOM</b>	3473 CD LYS B 520	52.251 31.565 79.419 1.00 59.42	С
<b>ATOM</b>	3474 CE LYS B 520	52.759 32.291 80.663 1.00 64.54	С
<b>ATOM</b>	3475 NZ LYS B 520	53.052 31.377 81.814 1.00 65.32	N
<b>ATOM</b>	3476 N GLY B 521	47.908 28.460 78.487 1.00 41.64	N
<b>ATOM</b>	3477 CA GLY B 521	46.982 27.422 78.792 1.00 38.71	С
<b>ATOM</b>	3478 C GLY B 521	47.455 26.053 78.433 1.00 38.07	С
<b>ATOM</b>	3479 O GLY B 521	47.258 25.105 79.160 1.00 38.25	0
<b>ATOM</b>	3480 N MET B 522	48.115 25.848 77.306 1.00 42.81	N
	3481 CA MET B 522	48.619 24.507 76.999 1.00 45.50	С
	3482 C MET B 522	49.656 24.090 78.013 1.00 50.52	С
ATOM		49.557 22.956 78.456 1.00 56.62	O
	3484 CB MET B 522	49.239 24.413 75.630 1.00 40.58	С
	3485 CG MET B 522	48.145 24.744 74.627 1.00 43.42	С

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			101/371	
<b>ΛΤΩΜ</b>	3.186	SD_MET R.522	48.718 24.184 73.023 1.00 48.78	S
ATOM	3.187	CE MET B 522	47.330 24.747 72.036 1.00 46.57	Č
ATOM	3488	N GILLR 523	50.529 24.985 78.435 1.00 56.27	N
			51.544 24.685 79.459 1.00 59.59	
			50.800 24.081 80.664 1.00 61.35	
ATOM	3491	O GLUB 523	51.112 23.012 81.125 1.00 62.06	Ö
ATOM	3492	CB GLU B 523	52.236 25.939 79.934 1.00 60.48	C
			53.692 26.141 80.004 1.00 62.32	
			54.189 27.545 79.761 1.00 65.44	
ATOM	3105	OE1 GLUB 523	54 319 28 008 78 588 1 00 68 32	0
ATOM	3496	OE2 GLU B 523	54.460 28.254 80.746 1.00 66.60	0
ATOM	3497	N HIS B 524	49.819 24.808 81.137 1.00 65.14	N
			48.998 24.437 82.275 1.00 69.75	С
ATOM	3499	C HIS B 524	48.255 23.145 82.016 1.00 69.68	C
ATOM	3500	O HIS B 524	48.273 22.235 82.845 1.00 67.93	0
ATOM	3501	CB HIS B 524	48.273 22.235 82.845 1.00 67.93 48.048 25.598 82.574 1.00 73.34 47.051 25.312 83.628 1.00 77.40 45.809 25.918 83.647 1.00 79.82	<b>C</b>
ATOM	3502	CG HIS B 524	47.051 25.312 83.628 1.00 77.40	С
ATOM	3503	ND1 HIS B 524	45.809 25.918 83.647 1.00 79.82	N
ATOM	3504	CD2 HIS B 524	47.105 24.488 84.700 1.00 79.32	C
ATOM	3505	CE1 HIS B 524	45.125 25.493 84.701 1.00 80.73	С
ATOM	3506	NE2 HIS B 524	45.894 24.624 85.344 1.00 82.59	N
			47.715 22.983 80.812 1.00 70.58	
			47.028 21.725 80.538 1.00 74.84	
			48.035 20.582 80.642 1.00 79.93	
ATOM	3510	O LEU B 525	47.759 19.633 81.377 1.00 81.47	0
ATOM	3511	CB LEU B 525	46.341 21.724 79.198 1.00 73.42	C
ATOM	3512	CG LEU B 525	44.836 21.743 79.060 1.00 71.12 44.148 22.671 80.045 1.00 70.99	
ATOM	3313	CD1 LEU B 525	44.148 22.071 80.045 1.00 70.99	C
			44.459 22.156 77.636 1.00 71.27 49.165 20.643 79.958 1.00 84.77	
ATOM	2516	CA TVD D 526	50.153 19.579 80.005 1.00 91.06	C
			50.835 19.399 81.335 1.00 92.45	
		O TYR B 526	51.138 18.252 81.737 1.00 92.79	0
		CB TYR B 526	51.147 19.722 78.849 1.00 95.73	C
		CG ATYR B 526	50.422 19.566 77.521 0.50 97.65	C
		CG BTYR B 526	52.174 18.632 78.708 0.50 98.64	č
		CD1ATYR B 526		Ċ
		CD1BTYR B 526	52.083 17.432 79.396 0.50100.15	C
		CD2ATYR B 526		С
		CD2BTYR B 526	53.272 18.779 77.859 0.50 99.84	С
		CE1ATYR B 526	49.514 18.159 75.788 0.50 99.35	С
		CE1BTYR B 526	53.002 16.422 79.294 0.50101.42	С
		CE2ATYR B 526	49.239 20.528 75.647 0.50 99.04	С
		CE2BTYR B 526	54.213 17.772 77.733 0.50101.17	С
ATOM	3530	CZ ATYR B 526	49.040 19.268 75.129 0.50 99.38	С
		CZ BTYR B 526	54.075 16.603 78.446 0.50101.98	С
		OH ATYR B 526	48.354 19.121 73.949 0.50100.58	Ο
		OH BTYR B 526	55.016 15.607 78.310 0.50103.74	Ο
ATOM	3534	N SER B 527	50.986 20.432 82.151 1.00 93.82	N

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51.517	20.212

			51.517 20.212 83.504 1.00 96.43	С
			50.635 19.206 84.243 1.00 99.93	С
<b>ATOM</b>	3537	O SER B 527	51.122 18.212 84.783 1.00 99.91	0
ATOM	3538	CB SER B 527	51.654 21.528 84.228 1.00 95.12	С
ATOM	3539	OG SER B 527	50.575 21.842 85.055 1.00 93.84	0
ATOM	3540	N MET B 528	49.324 19.442 84.235 1.00104.05	N
ATOM	3541	CA MET B 528	48.348 18.580 84.874 1.00106.28	С
ATOM	3542	C MET B 528	48.514 17.114 84.501 1.00109.30	С
ATOM	3543	O MET B 528	49.146 16.375 85.280 1.00110.26	Ο
ATOM	3544	CB MET B 528	46.934 19.066 84.578 1.00104.92	С
ATOM	3545	CG MET B 528	46.616 20.428 85.186 1.00103.89	С
<b>ATOM</b>	3546	SD MET B 528	45.067 21.090 84.521 1.00102.69	S
<b>ATOM</b>	3547	CE MET B 528	43.976 19.685 84.768 1.00103.03	С
ATOM	3548	N LYS B 529	47.979 16.659 83.392 1.00112.58	N
ATOM	3549	CA LYS B 529	47.968 15.274 82.952 1.00114.66	С
<b>ATOM</b>	3550	C LYS B 529	46.519 14.757 82.954 1.00115.44	С
<b>ATOM</b>	3551	O LYS B 529	46.210 13.626 83.307 1.00115.58	Ο
ATOM	3552	CB LYS B 529	48.833 14.322 83.758 1.00115.06	С
<b>ATOM</b>	3553	N LEU B 536	47.047 14.467 69.426 1.00 90.47	N
ATOM	3554	CA LEUB 536	45.800 15.110 68.992 1.00 91.19	С
<b>ATOM</b>	3555	C LEU B 536	45.806 15.246 67.479 1.00 90.41	С
<b>ATOM</b>	3556	O LEU B 536	44.762 15.397 66.845 1.00 91.34	0
ATOM	3557	CB LEUB 536	45.635 16.485 69.635 1.00 90.56	С
<b>ATOM</b>	3558	CG LEUB 536	44.545 17.411 69.144 1.00 89.27	C
<b>ATOM</b>	3559	CD1 LEU B 536	43.162 16.805 69.074 1.00 89.56	С
<b>ATOM</b>	3560	CD2 LEU B 536	44,632 18,761 69,813 1,00 88,59	С
<b>ATOM</b>	3561	N TYR B 537	47.016 15.149 66.935 1.00 91.03	N
<b>ATOM</b>	3562	CA TYR B 537	47.194 15.255 65.492 1.00 91.03	С
<b>ATOM</b>	3563	C TYR B 537	46.231 14.307 64.787 1.00 90.74	С
<b>ATOM</b>	3564	O TYR B 537	45.467 14.712 63.911 1.00 89.89	O
ATOM	3565	CB TYR B 537	48.651 14.949 65.101 1.00 90.58	С
		CG TYR B 537		С
<b>ATOM</b>	3567	CD1 TYR B 537	48.486 14.030 62.760 1.00 91.31	С
<b>ATOM</b>	3568	CD2 TYR B 537	49,323 16.251 63.041 1.00 92.16	С
<b>ATOM</b>	3569	CE1 TYR B 537	48.636 14.149 61.396 1.00 93.25	C
		CE2 TYR B 537	49.481 16.379 61.672 1.00 92.69	C
		CZ TYR B 537	49.134 15.324 60.855 1.00 93.50	С
		OH TYR B 537	49.265 15.403 59.485 1.00 93.62	O
		N ASP B 538	46.306 13.033 65.173 1.00 91.50	N
<b>ATOM</b>	3574	CA ASP B 538	45.486 11.989 64.559 1.00 92.46	С
<b>ATOM</b>	3575	C ASP B 538	44.045 12.098 65.027 1.00 89.47	С
		O ASP B 538	43.116 11.887 64.239 1.00 89.78	0
		CB ASP B 538	46.059 10.611 64.812 1.00 96.58	С
ATOM	3578	CG ASP B 538	47.466 10.656 65.393 1.00 98.56	С
<b>ATOM</b>	3579	OD1 ASP B 538	48.385 11.085 64.658 1.00 98.61	О
		OD2 ASP B 538	47.567 10.262 66.578 1.00100.00	0
		N LEU B 539	43.860 12.515 66.285 1.00 85.65	N
		CA LEUB 539	42.515 12.744 66.774 1.00 82.51	С
ATOM	3583	C LEU B 539	41.753 13.616 65.771 1.00 79.45	С

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ATOM	3584 C	D LEU B 539	40.688 13.197 65.351 1.00 77.96	Ο
			42,444 13,387 68,160 1,00 83,22	С
ATOM	3586 C	CG LEUB 539	40.995 13.548 68.674 1.00 84.94	С
ATOM			40.178 12.277 68.459 1.00 84.31	С
			40.886 13.991 70.123 1.00 84.23	С
			42.333 14.748 65.377 1.00 76.53	N
ATOM			41.691 15.629 64.394 1.00 74.04	С
		<del>-</del> · ·	41.634 15.010 63.008 1.00 72.97	С
			40.703 15.130 62.207 1.00 67.85	Ο
			42.448 16.976 64.343 1.00 69.75	С
			42.627 17.636 65.710 1.00 67.68	С
			43.630 18.774 65.641 1.00 67.75	С
			41.288 18.127 66.240 1.00 66.55	C
			42.734 14.308 62.684 1.00 74.85	N
			42.817 13.660 61.369 1.00 75.55	C
			41.604 12.757 61.179 1.00 74.33	c
			40.915 12.818 60.174 1.00 73.71	Ö
			44.101 12.859 61.270 1.00 76.52	C
			44.429 12.193 59.942 1.00 77.83	Č
			43.682 12.832 58.761 1.00 77.63	C
			45.937 12.242 59.708 1.00 76.18	C
ATOM			41.323 11.945 62.184 1.00 74.70	N
ATOM			40.161 11.055 62.111 1.00 78.10	Ċ
ATOM			38.871 11.830 62.028 1.00 76.88	c
			38.025 11.609 61.165 1.00 76.15	Ö
ATOM			40.206 10.099 63.314 1.00 81.69	C
			41.236 8.981 63.062 1.00 86.31	c
			40.967 8.283 61.729 1.00 90.86	č
			39.878 7.669 61.534 1.00 92.07	Ö
			41.868 8.367 60.853 1.00 92.44	Ö
			38.753 12.820 62.890 1.00 76.90	N
			37.654 13.758 62.973 1.00 77.35	Ĉ
				C
			37.421 14.492 61.665 1.00 76.40	Ö
		O MET B 543		C
		CB MET B 543	38.008 14.769 64.083 1.00 79.63 38.041 14.163 65.465 1.00 80.33	C
		CG MET B 543	37.001 15.039 66.655 1.00 83.37	S
		SD MET B 543		C
		CE MET B 543	38.090 14.960 68.082 1.00 80.57	N
		N LEUB 544	38.514 14.931 61.037 1.00 78.72	C
			38.450 15.633 59.761 1.00 80.40	
		C LEU B 544	38.116 14.649 58.643 1.00 86.77	C
		O LEUB 544	37.409 14.973 57.688 1.00 85.08	0
		CB LEUB 544	39.762 16.355 59.539 1.00 75.21	C
		CG LEUB 544	39.822 17.785 60.068 1.00 72.72	C
			41.249 18.270 60.143 1.00 70.71	C
		CD2 LEU B 544	38.970 18.702 59.200 1.00 72.37	C
		N ASP B 545	38.582 13.412 58.826 1.00 94.59	N
			38.296 12.264 57.997 1.00101.77	C
ATOM	3632 (	C ASP B 545	36.804 11.881 58.061 1.00103.94	С

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ATOM 3681 NE2 HIS B 550 31.180 11.617 62.283 1.00132.12 N ATOM 3682 N ALA B 551 26.545 12.411 58.645 1.00138.08 N ATOM 3683 CA ALA B 551 25.256 12.796 58.080 1.00138.49 C ATOM 3684 C ALA B 551 24.858 14.189 58.542 1.00138.87 C ATOM 3685 O ALA B 551 25.318 15.156 57.901 1.00139.61 O ATOM 3686 CB ALA B 551 24.215 11.761 58.460 1.00139.09 C TER 3687 ALA B 551 HETATM 3688 C1 CBM B 381 50.363 23.182 66.508 1.00 70.74 C HETATM 3689 C2 CBM B 381 50.898 24.501 67.006 1.00 63.90 C	<b>ATOM</b>	3679	CD2 HIS B 550	30.522 11.529 61.086 1.00132.55	
ATOM 3682 N ALAB 551 26.545 12.411 58.645 1.00138.08 N ATOM 3683 CA ALAB 551 25.256 12.796 58.080 1.00138.49 C ATOM 3684 C ALAB 551 24.858 14.189 58.542 1.00138.87 C ATOM 3685 O ALAB 551 25.318 15.156 57.901 1.00139.61 O ATOM 3686 CB ALAB 551 24.215 11.761 58.460 1.00139.09 C TER 3687 ALAB 551 HETATM 3688 C1 CBM B 381 50.363 23.182 66.508 1.00 70.74 C HETATM 3689 C2 CBM B 381 50.898 24.501 67.006 1.00 63.90 C	<b>ATOM</b>	3680	CE1 HIS B 550	31.219 12.880 62.652 1.00132.14	С
ATOM 3683 CA ALAB 551 25.256 12.796 58.080 1.00138.49 C ATOM 3684 C ALAB 551 24.858 14.189 58.542 1.00138.87 C ATOM 3685 O ALAB 551 25.318 15.156 57.901 1.00139.61 O ATOM 3686 CB ALAB 551 24.215 11.761 58.460 1.00139.09 C TER 3687 ALAB 551 HETATM 3688 C1 CBM B 381 50.363 23.182 66.508 1.00 70.74 C HETATM 3689 C2 CBM B 381 50.898 24.501 67.006 1.00 63.90 C	<b>ATOM</b>	3681	NE2 HIS B 550	31.180 11.617 62.283 1.00132.12	N
ATOM 3684 C ALA B 551 24.858 14.189 58.542 1.00138.87 C ATOM 3685 O ALA B 551 25.318 15.156 57.901 1.00139.61 O ATOM 3686 CB ALA B 551 24.215 11.761 58.460 1.00139.09 C TER 3687 ALA B 551 HETATM 3688 C1 CBM B 381 50.363 23.182 66.508 1.00 70.74 C HETATM 3689 C2 CBM B 381 50.898 24.501 67.006 1.00 63.90 C	<b>ATOM</b>	3682	N ALA B 551	26.545 12.411 58.645 1.00138.08	N
ATOM 3685 O ALAB 551 25.318 15.156 57.901 1.00139.61 O ATOM 3686 CB ALAB 551 24.215 11.761 58.460 1.00139.09 C TER 3687 ALAB 551 HETATM 3688 C1 CBM B 381 50.363 23.182 66.508 1.00 70.74 HETATM 3689 C2 CBM B 381 50.898 24.501 67.006 1.00 63.90 C	<b>ATOM</b>	3683	CA ALAB 551	25.256 12.796 58.080 1.00138.49	С
ATOM 3686 CB ALAB 551 24.215 11.761 58.460 1.00139.09 C TER 3687 ALAB 551 HETATM 3688 C1 CBM B 381 50.363 23.182 66.508 1.00 70.74 C HETATM 3689 C2 CBM B 381 50.898 24.501 67.006 1.00 63.90 C	<b>ATOM</b>	3684	C ALA B 551	24.858 14.189 58.542 1.00138.87	С
ATOM 3686 CB ALAB 551 24.215 11.761 58.460 1.00139.09 C TER 3687 ALAB 551 HETATM 3688 C1 CBM B 381 50.363 23.182 66.508 1.00 70.74 C HETATM 3689 C2 CBM B 381 50.898 24.501 67.006 1.00 63.90 C				25.318 15.156 57.901 1.00139.61	O
TER 3687 ALA B 551  HETATM 3688 C1 CBM B 381 50.363 23.182 66.508 1.00 70.74 C  HETATM 3689 C2 CBM B 381 50.898 24.501 67.006 1.00 63.90 C					С
HETATM 3688 C1 CBM B 381 50.363 23.182 66.508 1.00 70.74 C HETATM 3689 C2 CBM B 381 50.898 24.501 67.006 1.00 63.90 C					
HETATM 3689 C2 CBM B 381 50.898 24.501 67.006 1.00 63.90 C				1 50.363 23.182 66.508 1.00 70.74	С
					С
					О

V. 2	105 (371	
1777 173 4 3 6 0 1 0 0 CD3 4 D 3 0 1	50 150 22 250 67 200 1 00 72 88	0
HETATM 3691 O2 CBM B 381	50.159 22.259 67.288 1.00 73.88	0
HETATM 3692 C1 RAL B 600	37.136 24.786 77.943 1.00 41.59	C
HETATM 3693 C2 RAL B 600	36.077 25.070 77.112 1.00 39.83	C
HETATM 3694 C3 RAL B 600	35.957 26.328 76.578 1.00 38.16	C
HETATM 3695 O3 RAL B 600	34.871 26.528 75.754 1.00 40.43	O
HETATM 3696 C4 RAL B 600	36.882 27.310 76.907 1.00 39.29	C
HETATM 3697 C5 RAL B 600	37.925 27.033 77.738 1.00 39.54	С
HETATM 3698 S6 RAL B 600	39.146 28.022 78.355 1.00 40.30	S
HETATM 3699 C7 RAL B 600	39.970 26.805 79.208 1.00 41.19	С
HETATM 3700 C8 RAL B 600	41.199 27.019 80.019 1.00 39.95	С
HETATM 3701 C9 RAL B 600	41.345 28.185 80.728 1.00 41.84	С
HETATM 3702 C10 RAL B 600	42.438 28.411 81.548 1.00 44.69	С
HETATM 3703 C11 RAL B 600	43,437 27,448 81,612 1,00 45,99	С
HETATM 3704 O11 RAL B 600	44.521 27.695 82.432 1.00 50.33	Ō
HETATM 3705 C12 RAL B 600	43.314 26.290 80.885 1.00 42.47	Ċ
HETATM 3706 C13 RAL B 600	42.179 26.085 80.108 1.00 39.90	C
HETATM 3707 C14 RAL B 600	38.054 25.738 78.252 1.00 38.16	C
HETATM 3708 C15 RAL B 600	39.227 25.613 79.090 1.00 38.60	č
HETATM 3709 C16 RAL B 600	39.540 24.434 79.718 1.00 37.47	Č
HETATM 3710 O16 RAL B 600	39.634 24.372 80.932 1.00 36.58	Ö
HETATM 3711 C17 RAL B 600	39.914 23.230 78.994 1.00 34.13	C
	39.972 22.094 79.765 1.00 34.73	C
HETATM 3712 C18 RAL B 600		C
HETATM 3713 C19 RAL B 600	40.396 20.876 79.214 1.00 34.59	C
HETATM 3714 C20 RAL B 600	40.771 20.895 77.901 1.00 38.96	
HETATM 3715 C21 RAL B 600	40.752 22.057 77.116 1.00 37.83	C
HETATM 3716 C22 RAL B 600	40.305 23.245 77.679 1.00 35.52	C
HETATM 3717 O23 RAL B 600	41.204 19.791 77.200 1.00 44.41	0
HETATM 3718 C24 RAL B 600	40.319 18.706 77.123 1.00 45.36	C
HETATM 3719 C25 RAL B 600	41.196 17.625 76.411 1.00 44.46	C
HETATM 3720 N26 RAL B 600	40.895 17.562 74.984 1.00 43.60	N
HETATM 3721 C27 RAL B 600	41.659 16.562 74.294 1.00 43.45	C
HETATM 3722 C28 RAL B 600	41.488 16.507 72.779 1.00 44.58	С
HETATM 3723 C29 RAL B 600		C
HETATM 3724 C30 RAL B 600	40.388 18.722 72.842 1.00 45.78	С
HETATM 3725 C31 RAL B 600		С
HETATM 1 O HOH 1 78.	.671 45.635 73.728 1.00 18.41	
HETATM 2 O HOH 2 65.	.939 43.852 69.249 1.00 23.40	
<b>HETATM</b> 3 O HOH 3 67.	.879 41.641 69.144 1.00 32.98	
HETATM 4 O HOH 4 72.	.161 43.516 68.328 1.00 32.96	
HETATM 5 O HOH 5 45.	.293 41.236 55.063 1.00 36.48	
HETATM 6 O HOH 6 49.	.117 45.566 50.606 1.00 44.30	
HETATM 7 O HOH 7 66.	.937 34.473 57.692 1.00 38.73	
HETATM 8 O HOH 8 69.	.523 44.664 70.139 1.00 37.12	
	.684 41.492 67.111 1.00 46.69	
	2.332 42.566 71.041 1.00 39.72	
	7.230 47.810 75.360 1.00 41.93	
	8.753 44.504 65.387 1.00 47.61	
	6.079 37.937 81.002 1.00 48.27	
	0.480 45.943 67.468 1.00 53.17	

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106/371 56,336 35,571 76,185 1,00 44,22 HETATM 15 O HOH 15 40.293 54.526 68.285 1.00 65.88 HETATM 16 O HOH 16 48.191 42.643 49.929 1.00 66.50 HETATM 17 O HOH 17 HETATM 18 O HOH 18 42.953 57.811 69.507 1.00 88.95 **НЕТАТМ 19 О НОН** 19 66.169 45.843 67.240 1.00 30.54 HETATM 20 O HOH 20 63.477 52.158 67.006 1.00 37.54 79.511 32.798 62.361 1.00 58.45 HETATM 21 O HOH 21 HETATM 22 O HOH 22 79.665 44.463 70.700 1.00 50.89 HETATM 23 O HOH 23 59.043 57.930 76.285 1.00 75.57 60,390 37,277 84,122 1.00 43,42 HETATM 24 O HOH 24 HETATM 25 O HOH 25 76.899 29.211 59.311 1.00 72.06 53.280 40.076 69.802 1.00 43.07 HETATM 26 O HOH 26 HETATM 27 O HOH 27 45,293 51,300 66,697 1,00 40,03 47.486 57.944 58.839 1.00 56.99 HETATM 28 O HOH 28 HETATM 29 O HOH 29 47.155 44.689 45.733 1.00 81.53 48.375 39.816 66.498 1.00 50.55 HETATM 30 O HOH 30 HETATM 31 O HOH 31 54.862 44.533 76.824 1.00 38.59 81,320 34,485 67,792 1.00 53.56 HETATM 32 O HOH 32 HETATM 33 O HOH 78.189 37.052 73.346 1.00 55.28 33 59.058 38.545 75.613 1.00 27.41 HETATM 34 O HOH 34 56.115 30.116 78.032 1.00 64.88 HETATM 35 O HOH 35 48.376 56.369 48.335 1.00 74.84 HETATM 36 O HOH 36 45.334 56.547 54.616 1.00 51.79 HETATM 37 O HOH 37 HETATM 38 O HOH 68.751 46.528 72.429 1.00 61.72 38 39 68.749 48.138 63.262 1.00 75.75 HETATM 39 O HOH 40 71.042 50.167 64.313 1.00 57.30 HETATM 40 O HOH HETATM 41 O HOH 41 51.867 54.038 84.504 1.00 55.62 HETATM 42 O HOH 42 46.423 34.649 68.035 1.00 59.90 43 65.977 46.032 71.358 1.00 39.14 HETATM 43 O HOH 44 51.878 43.672 50.996 1.00 56.18 HETATM 44 O HOH 80.471 31.343 76.488 1.00 42.36 45 HETATM 45 O HOH 71.303 44.041 59.439 1.00 70.71 HETATM 46 O HOH 46 41.452 53.507 71.888 1.00 75.54 HETATM 47 O HOH 47 HETATM 48 O HOH 82.937 41.654 71.088 1.00 75.67 48 HETATM 49 O HOH 65,172 34,557 81.617 1.00 57.84 49 67.048 50.080 60.811 1.00 49.02 HETATM 50 O HOH 50 HETATM 51 O HOH 51 55,298 50,332 52,676 1,00 48,09 HETATM 52 O HOH 56,566 48,350 50,527 1.00 62,34 52 HETATM 53 O HOH 69.733 31.591 80.417 1.00 84.65 53 HETATM 54 O HOH 54 54.694 40.240 86.738 1.00 70.28 HETATM 55 O HOH 59.333 24.933 73.595 1.00 57.45 55 HETATM 56 O HOH 56 70.409 51.391 81.779 1.00 59.24 31.845 31.472 62.530 1.00 29.20 HETATM 1 O HOH 57 HETATM 2 O HOH 58 32.562 30.513 69.296 1.00 34.69 HETATM 3 O HOH 59 34.498 28.884 70.461 1.00 29.20 HETATM 4 O HOH 60 45,409 26,911 70,363 1,00 32,57 HETATM 5 O HOH 61 34.193 27.990 73.282 1.00 30.58 62 32.822 24.241 68.673 1.00 40.19 HETATM 6 O HOH HETATM 7 O HOH 33.935 27.969 65.961 1.00 35.49 63

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HETATM	8 O	HOH	64	30.796 19.159 80.905 1.00 50.10
HETATM	9 O	HOH	65	29.988 26.357 73.687 1.00 40.36
HETATM	10 O	HOH	66	46.316 34.186 65.148 1.00 39.13
HETATM	$\Pi$ 0	НОН	67	30.697 30.965 71.805 1.00 50.24
HETATNI	12 O	НОН	68	49.113 27.839 71.457 1.00 47.01
<b>HETATM</b>	13 O	HOH	69	40.944 40.126 48.862 1.00 55.13
HETATM	i4 O	нон	70	32.119 26.221 70.754 1.00 51.01
HETATM	15 O	HOH	71	37.406 41.975 48.996 1.00 47.12
HETATM	16 O	HOH	72	48.657 39.247 50.483 1.00 63.81
HETATM	17 O	НОН	73	26.862 41.181 48.762 1.00 69.42
HETATM	is O	НОН	74	25.401 30.214 67.857 1.00 72.19
HETATM	19 O	HOH	75	30.576 21.546 58.202 1.00 51.83
<b>HETATM</b>	20 O	HOH	76	35.909 14.132 78.132 1.00 62.99
HETATM	21 O	HOH	<b>77</b>	52.634 29.330 63.071 1.00 58.31
HETATM	22 O	HOH	78	26.808 27.051 57.128 1.00 45.94
HETATM	23 O	HOH	79	29.245 28.608 55.705 1.00 83.48
HETATM	24 O	HOH	80	29.129 27.091 76.317 1.00 33.47
HETATNI	25 O	HOH	81	33.625 38.647 81.633 1.00 41.20
HETATNI	26 O	HOH	82	36.603 51.147 53.895 1.00 48.15
HETATM	27 O	НОН	83	28.622 46.426 60.451 1.00 52.33
HETATM	28 O	HOH	84	38.056 53.295 65.884 1.00 60.11
HETATM	29 O	HOH	85	43.521 38.970 58.179 1.00 51.73
HETATN	30 O	HOH	86	27.777 37.624 76.264 1.00 70.19
HETATM	31 O	HOH	87	22.739 30.334 60.747 1.00 67.64
HETATM	32 O	HOH	88	26.762 28.420 86.838 1.00 65.95
HETATN	33 O	HOH	89	39.032 29.779 46.494 1.00 89.14
HETATN	34 O	HOH	90	34.718 26.674 68.385 1.00 47.22
HETATM	35 O	HOH	91	29.738 28.093 71.095 1.00 44.84
HETATM	36 O	HOH	92	55.506 30.331 64.286 1.00 70.99
HETATM	37 O	HOH	93	29.692 12.806 76.719 1.00 53.32
HETATNI	38 O	HOH	94	29.342 24.024 63.816 1.00 67.83
HETATM	39 O	HOH		29.596 43.489 50.236 1.00 55.40
HETATNI	40 O	HOH	96	33.505 15.266 63.104 1.00 76.39
HETATM	41 O	HOH	97	36.057 14.492 70.938 1.00 71.41
HETATNI	42 O	HOH	98	26.881 34.813 73.143 1.00 72.62
HETATNI	43 O	HOH	99	27.506 35.250 67.027 1.00 53.58
HETATNI	44 O	HOH	100	25.166 33.321 65.780 1.00 85.60
END				

## FIGURE 21

08-SEP-97 1ERE HEADER NUCLEAR RECEPTOR TITLE HUMAN OESTROGEN RECEPTOR LIGAND-BINDING DOMAIN IN COMPLEX TITLE 2 WITH 17BETA-OESTRADIOL COMPND MOL ID: 1; COMPND 2 MOLECULE: OESTROGEN RECEPTOR; COMPND 3 CHAIN: A, B, C, D, E, F; COMPND 4 FRAGMENT: LIGAND-BINDING DOMAIN; COMPND 5 SYNONYM: ESTROGEN RECEPTOR, ER-LBD; COMPND 6 BIOLOGICAL\_UNIT: DIMER; COMPND 7 OTHER DETAILS: LIGAND-BINDING DOMAIN COMPND 8 (DOMAIN E - RESIDUES 301-553) IN COMPLEX WITH ENDOGENOUS COMPND 9 LIGAND 17BETA-OESTRADIOL SOURCE MOL ID: 1; SOURCE 2 ORGANISM\_SCIENTIFIC: HOMO SAPIENS; SOURCE 3 ORGANISM\_COMMON: HUMAN; SOURCE 4 STRAIN: JM109; SOURCE 5 VARIANT: C1857; SOURCE 6 PLASMID: PEALPHA 35; SOURCE 7 GENE: ER ALPHA KEYWDS , NUCLEAR RECEPTOR, TRANSCRIPTION FACTOR, STEROID, AGONIST AUTHOR A.M.BRZOZOWSKI, A.C.W.PIKE REMARK 1 REMARK 2 REMARK 2 RESOLUTION. 3.1 ANGSTROMS. REMARK 3 REMARK 3 REFINEMENT. REMARK 3 PROGRAM : REFMAC REMARK 3 AUTHORS : MURSHUDOV, VAGIN, DODSON REMARK 3 REMARK 3 DATA USED IN REFINEMENT. REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS): 3.1 REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS): 20 (SIGMA(F)): 0REMARK 3 DATA CUTOFF REMARK 3 COMPLETENESS FOR RANGE (%): 99.1 REMARK 3 NUMBER OF REFLECTIONS : 33981 REMARK 3 REMARK 3 FIT TO DATA USED IN REFINEMENT. REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT REMARK 3 FREE R VALUE TEST SET SELECTION: RANDOM REMARK 3 R VALUE (WORKING + TEST SET): NONE REMARK 3 R VALUE (WORKING SET): 0.218 REMARK 3 FREE R VALUE : 0.251

REMARK 3 FREE R VALUE TEST SET SIZE (%):10

REMARK 3 FREE R VALUE TEST SET COUNT : 3398

REMARK 3

REMARK 6 ER-LBD WAS CARBOXYMETHYLATED PRIOR TO CRYSTALLISATION

BUT

REMARK 5 MODIFIED CYSTEINES ARE NOT MODELLED IN THIS ENTRY.

REMARK 7

REMARK 7 RESIDUES LEU306, LEU466, LEU469, LYS492, LYS531 AND LEU536

REMARK 7 (CHAINS ABCDEF) WERE POORLY RESOLVED IN THE ELECTRON

REMARK 7 DENSITY MAPS AND ARE NOT FULLY MODELLED IN THIS ENTRY.

REMARK S

REMARK S RESIDUES MODELLED IN ALTERNATE CONFORMATIONS (CHAINS

**REMARK** 8 ABCDEF): 377,501,513,530

REMARK 399

REMARK 999 SEQUENCE

REMARK 999 REFERENCE: REFERENCE: SER A 301 - ASN A 304 MISSING FROM

REMARK 999 PDB DUE TO DISORDER TYR A 331 - PRO A 336 MISSING FROM

REMARK 999 PDB DUE TO DISORDER LEU A 462 - SER A 464 MISSING FROM

REMARK 999 PDB DUE TO DISORDER LEU A 549 - THR A 553 MISSING FROM

REMARK 999 PDB DUE TO DISORDER.

REMARK 999 REFERENCE: REFERENCE: SER B 301 - ASN B 304 MISSING FROM

REMARK 999 PDB DUE TO DISORDER TYR B 331 - PRO B 336 MISSING FROM

REMARK 999 PDB DUE TO DISORDER LEU B 462 - SER B 464 MISSING FROM

REMARK 999 PDB DUE TO DISORDER LEU B 549 - THR B 553 MISSING FROM

REMARK 999 PDB DUE TO DISORDER.

REMARK 999 REFERENCE: REFERENCE: SER C 301 - ASN C 304 MISSING FROM

REMARK 999 PDB DUE TO DISORDER TYR C 331 - PRO C 336 MISSING FROM

REMARK 999 PDB DUE TO DISORDER LEU C 462 - SER C 464 MISSING FROM

REMARK 999 PDB DUE TO DISORDER LEU C 549 - THR C 553 MISSING FROM

REMARK 999 PDB DUE TO DISORDER. REMARK 999 REFERENCE: REFERENCE: SER D 301 - ASN D 304 MISSING FROM REMARK 999 PDB DUE TO DISORDER TYR D 331 - PRO D 336 MISSING FROM REMARK 999 PDB DUE TO DISORDER LEU D 462 - SER D 464 MISSING FROM REMARK 999 PDB DUE TO DISORDER LEU D 549 - THR D 553 MISSING FROM REMARK 999 PDB DUE TO DISORDER. REMARK 999 REFERENCE: REFERENCE: SER E 301 - ASN E 304 MISSING FROM REMARK 999 PDB DUE TO DISORDER TYR E 331 - PRO E 336 MISSING FROM REMARK 999 PDB DUE TO DISORDER LEU E 462 - SER E 464 MISSING FROM REMARK 999 PDB DUE TO DISORDER LEU E 549 - THR E 553 MISSING FROM REMARK 999 PDB DUE TO DISORDER. REMARK 999 REFERENCE: REFERENCE: SER F 301 - ASN F 304 MISSING FROM REMARK 999 PDB DUE TO DISORDER TYR F 331 - PRO F 336 MISSING FROM REMARK 999 PDB DUE TO DISORDER LEU F 462 - SER F 464 MISSING FROM REMARK 999 PDB DUE TO DISORDER LEU F 549 - THR F 553 MISSING FROM REMARK 999 PDB DUE TO DISORDER. CRYST1 61.480 115.160 137.380 90.00 98.80 90.00 P 1 21 1 12 ORIGX1 1.000000 0.000000 0.000000 0.00000 0.000000 1.000000 0.000000 ORIGX2 0.00000 ORIGX3 0.000000 0.000000 1.000000 0.00000 0.016265 0.000000 0.002518 SCALE 0.00000 0.000000 0.008684 0.000000 SCALE2 0.00000

0.000000 0.000000 0.007366 SCALE3 0.00000 N ATOM 1 N SER A 305 22.376 70.539 109.257 1.00 90.58 21.381 69.729 110.019 1.00 89.92 ATOM 2 CA SER A 305 C 3 C SER A 305 ATOM 20.264 70.593 110.587 1.00 89.41 C 0 ATOM 4 O SER A 305 20.539 71.556 111.320 1.00 89.09 22.072 68.944 111.149 1.00 89.79 ATOM 5 CB SER A 305 C 0 ATOM 6 OG SER A 305 21.136 68.215 111.938 1.00 89.19 7 N LEU A 306 19.015 70.206 110.299 1.00 88.77 N ATOM 8 CA LEU A 306 17.865 70.930 110.863 1.00 88.07 C ATOM 9 C LEU A 306 18.131 71.087 112.365 1.00 86.68 C ATOM 0 ATOM 10 O LEU A 306 18.154 72.187 112.907 1.00 86.51

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C

C 16.542 70.192 110.645 1.00 88.32 11 CB LEU A 306 ATOM N 18,397 69,974 113,039 1,00 84:80 15 N ALA A 307 **ATOM** 18.729 69.938 114.436 1.00 83.76 C **ATOM** 16 CA ALA A 307 C 19.481 71.204 114.826 1.00 83.39 17 C ALA A 307 **ATOM** 0 18 O ALA A 307 18.990 71.996 115.641 1.00 83.52 **ATOM** C 19.658 68.756 114.709 1.00 84.44 19 CB ALA A 307 **ATOM** N 20.651 71.396 114.216 1.00 82.63 20 N LEU A 308 **ATOM** 21.450 72.573 114.519 1.00 82.87 C 21 CA LEU A 308 **ATOM** C 20.880 73.922 114.137 1.00 83.17 22 C LEU A 308 **ATOM** 21,524 74,938 114,470 1.00 85.07 0 23 O LEUA 308 **ATOM** 22.856 72.405 113.918 1.00 82.50 C 24 CB LEU A 308 **ATOM** 23.622 71.169 114.406 1.00 82.65 C **ATOM** 25 CG LEU A 308 25.115 71.374 114.134 1.00 82.32 C 26 CD1 LEU A 308 **ATOM** 23,409 70,923 115,910 1.00 82,67 C 27 CD2 LEU A 308 ATOM 19.730 74.056 113.506 1.00 82.11 N 28 N SER A 309 **ATOM** C 19.152 75.332 113.145 1.00 81.35 29 CA SER A 309 ATOM 17.899 75.697 113.915 1.00 79.81 C ATOM 30 C SER A 309 17.635 76.897 114.084 1.00 80.42 O ATOM 31 O SER A 309 18.766 75.242 111.654 1.00 83.07 C 32 CB SER A 309 ATOM 0 19.898 74.642 110.994 1.00 85.37 **ATOM** 33 OG SER A 309 17.120 74.699 114.355 1.00 77.25 N 34 N LEU A 310 ATOM 15.904 75.058 115.082 1.00 74.54 C **ATOM** 35 CA LEU A 310 16.256 75.861 116.330 1.00 73.69 C 36 C LEU A 310 ATOM 17.351 75.858 116.884 1.00 73.90 0 37 O LEU A 310 **ATOM** 15.045 73.869 115.438 1.00 74.07 C 38 CB LEU A 310 **ATOM** 15.143 72.689 114.475 1.00 74.30 C 39 CG LEU A 310 **ATOM** 15.798 71.520 115.196 1.00 74.63 C 40 CD1 LEU A 310 **ATOM** 13.775 72.311 113.936 1.00 74.41 C 41 CD2 LEU A 310 ATOM 15.256 76.611 116.750 1.00 72.43 N 42 N THR A 311 ATOM C 15.398 77.463 117.933 1.00 71.67 43 CA THR A 311 ATOM 14.918 76.624 119.094 1.00 70.84 C 44 C THR A 311 ATOM O 14.145 75.689 118.807 1.00 70.32 45 O THR A 311 ATOM C 46 CB THR A 311 14.566 78.734 117.727 1.00 72.13 ATOM 13.163 78.469 117.614 1.00 71.92 47 OG1 THR A 311 **ATOM** 14.993 79.395 116.418 1.00 72.78 48 CG2 THR A 311 ATOM N 15.271 76.947 120.334 1.00 70.12 49 N ALA A 312 ATOM C 14.791 76.149 121.458 1.00 69.91 50 CA ALA A 312 ATOM C 13.291 75.914 121.324 1.00 70.10 51 C ALA A 312 **ATOM** 0 12.840 74.799 121.594 1.00 70.35 52 O ALA A 312 ATOM C 53 CB ALA A 312 15.085 76.752 122.801 1.00 69.80 **ATOM** N 12.549 76.922 120.901 1.00 70.79 54 N ASP A 313 **ATOM** C 55 CA ASP A 313 11.123 76.716 120.726 1.00 72.57 **ATOM** C 56 C ASP A 313 10.756 75.706 119.664 1.00 70.70 **ATOM** 0 57 O ASP A 313 9.870 74.885 119.911 1.00 69.68 **ATOM** C 10.481 78.090 120.476 1.00 76.96 58 CB ASP A 313 **ATOM** 

13.114 67.526 122.055 1.00 50.58

C

**ATOM** 

103 CD1 LEU A 319

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ATOM	104 CD2 LEU A 319	12.767 65.812 120.232 1.00 50.24	C
ATOM	105 N LEU A 320		N
ATOM	106 CA LEU A 320	6.426 67.386 121.372 1.00 58.80	С
ATOM	107 C LEU A 320	5.587 66.689 120.321 1.00 61.20	С
ATOM	108 O LEU A 320	4.718 65.871 120.579 1.00 61.72	О
ATOM	109 CB LEU A 320	5.867 68.750 121.783 1.00 57.70	С
ATOM	110 CG LEU A 320	6.105 68.990 123.269 1.00 57.68	С
ATOM	111 CD1 LEU A 320	5.658 70.368 123.692 1.00 58.75	· C
ATOM	112 CD2 LEU A 320	5.402 67.915 124.081 1.00 57.28	C
ATOM	113 N ASP A 321	5.845 67.007 119.060 1.00 64.39	N
ATOM	114 CA ASP A 321	5.155 66.399 117.958 1.00 67.83	С
<b>ATOM</b>	115 C ASP A 321	5.484 64.951 117.672 1.00 66.45	С
ATOM	116 O ASP A 321	4.575 64.205 117.304 1.00 68.09	Ο
ATOM	117 CB ASP A 321	5.561 67.162 116.682 1.00 73.23	C
ATOM	118 CG ASP A 321	4.371 68.049 116.346 1.00 78.17	C
ATOM	119 OD1 ASP A 321	3.427 68.108 117.173 1.00 80.30	0
ATOM	120 OD2 ASP A 321	4.437 68.658 115.254 1.00 81.45	О
ATOM	121 N ALA A 322	6.742 64.551 117.828 1.00 62.92	N
<b>ATOM</b>	122 CA ALA A 322	7.106 63.176 117.533 1.00 59.78	С
ATOM	123 C ALA A 322		С
ATOM	124 O ALA A 322	6.491 60.986 118.187 1.00 58.35	О
ATOM	125 CB ALA A 322	8.623 63.125 117.574 1.00 59.62	С
ATOM	126 N GLU A 323	6.006 62.621 119.645 1.00 56.77	N
ATOM	127 CA GLU A 323		C
<b>ATOM</b>	128 C GLU A 323		C
ATOM	129 O GLU A 323	3.777 60.975 119.138 1.00 58.08	О
ATOM	130 CB GLU A 323	4.775 62.515 121.690 1.00 55.82	С
ATOM	131 CG GLU A 323	5.822 63.073 122.666 1.00 57.00	C
ATOM	132 CD GLU A 323		C
ATOM		5.500 61.285 124.241 1.00 57.59	0
ATOM		7.506 61.678 123.584 1.00 57.83	0
ATOM	135 N PRO A 324	4.769 59.403 120.344 1.00 55.05	N.
ATOM	136 CA PRO A 324		С
ATOM	137 C PRO A 324	2.646 58.236 120.586 1.00 54.98	C
ATOM	138 O PRO A 324	2.391 58.938 121.554 1.00 55.02	0
ATOM	139 CB PRO A 324	4.750 57.015 120.307 1.00 54.50	C
ATOM	140 CG PRO A 324	5.488 57.513 121.513 1.00 54.68	C
ATOM	141 CD PRO A 324	5.735 58.996 121.376 1.00 55.35	C
ATOM	142 N PRO A 325	1.758 57.400 120.099 1.00 56.07	N
ATOM	143 CA PRO A 325	0.428 57.188 120.623 1.00 56.86	C
ATOM	144 C PRO A 325	0.524 56.397 121.916 1.00 57.84	C
ATOM	145 O PRO A 325	1.583 55.785 122.033 1.00 58.89	0
ATOM	146 CB PRO A 325	-0.290 56.266 119.622 1.00 57.07	C
ATOM	147 CG PRO A 325	0.861 55.568 118.950 1.00 56.52	C
ATOM	148 CD PRO A 325	2.021 56.531 118.938 1.00 56.97	С
		•	

192 N PHE A 337

193 CA PHE A 337

-3.376 36.663 137.026 1.00 85.14

-1.980 37.049 136.956 1.00 85.09

N

C

ATOM

**ATOM** 

wo	98/56812	116/371	PCT/GB98/01708
ATOM	239 C MET A 343	4.863 38.836 130.511 1.00 57.16	C
<b>ATOM</b>	240 O MET A 343	5.226 39.762 129.786 1.00 58.46	0
<b>ATOM</b>	241 CB MET A 343	6.431 37.550 131.961 1.00 56.18	С
ATOM	242 CG MET A 343	7.321 37.682 133.190 1.00 56.31 8.204 39.248 133.273 1.00 56.60	С
	243 SD MET A 343	8.204 39.248 133.273 1.00 56.60	S
ATOM		8.874 39.359 131.604 1.00 55.24	C
		3.925 37.967 130.120 1.00 55.99	N
		3.273 38.073 128.833 1.00 53.83	C
ATOM		2.718 39.465 128.578 1.00 52.90	C
ATOM		3.122 40.066 127.583 1.00 53.02	0
ATOM		1.827 40.019 129.394 1.00 52.76	N C
ATOM	250 CA LEU A 345	1.305 41.347 129.094 1.00 53.20 2.394 42.408 128.910 1.00 52.33	c
ATOM	251 C LEU A 345	2.487 43.119 127.925 1.00 52.10	0
ATOM	252 O LEUA 343	0.464 41.917 130.219 1.00 54.25	C
ATOM ATOM		-0.848 41.244 130.534 1.00 55.33	C
ATOM		-0.756 40.738 131.968 1.00 56.61	C
ATOM		-1.953 42.272 130.348 1.00 55.75	Č
ATOM	257 N LEU A 346		N
ATOM		4.281 43.498 130.014 1.00 48.34	C
		5.124 43.395 128.760 1.00 47.59	C
ATOM	260 O LEU A 346	5 370 44 335 128,000 1,00 47,20	0
ATOM	261 CB LEU A 346	5.013 43.231 131.323 1.00 47.25 4.269 43.696 132.570 1.00 46.58 5.252 43.653 133.732 1.00 46.95	. <b>C</b>
ATOM	262 CG LEU A 346	4.269 43.696 132.570 1.00 46.58	<b>C</b> .
<b>ATOM</b>	263 CD1 LEU A 346	5.252 43.653 133.732 1.00 46.95	C
<b>ATOM</b>	264 CD2 LEU A 346	3.689 45.090 132.428 1.00 45.64	С
<b>ATOM</b>		5.556 42.174 128.487 1.00 46.40	N
<b>ATOM</b>	266 CA THR A 347	6.374 41.860 127.321 1.00 45.75	С
ATOM		5.697 42.169 126.020 1.00 46.81	C
ATOM		6.265 42.727 125.081 1.00 46.83	0
ATOM	•	6.733 40.397 127.565 1.00 45.43	C
ATOM	270 OG1 THR A 347	8.148 40.411 127.801 1.00 47.31	0
ATOM	271 CG2 THR A 347	6.253 39.444 126.535 1.00 44.20	C
ATOM	272 N ASN A 348	4.409 41.866 125.902 1.00 48.83	N
ATOM	273 CA ASN A 348	3.607 42.153 124.716 1.00 48.72	C
ATOM	274 C ASN A 348	3.511 43.662 124.507 1.00 47.34 3.719 44.247 123.449 1.00 47.88	C
ATOM ATOM	275 O ASN A 348 276 CB ASN A 348	2.210 41.560 124.918 1.00 51.06	C
ATOM	277 CG ASN A 348	1.272 41.891 123.765 1.00 54.34	C
ATOM	277 CG ASN A 348 278 OD1 ASN A 348	0.504 42.881 123.743 1.00 55.31	0
ATOM	279 ND2 ASN A 348	1.371 40.995 122.770 1.00 55.16	N
ATOM	280 N LEU A 349	3.194 44.396 125.563 1.00 45.51	N
ATOM	281 CA LEU A 349	3.045 45.841 125.500 1.00 43.88	C
ATOM	282 C LEU A 349	4.366 46.413 125.034 1.00 44.02	c
ATOM	283 O LEU A 349	4.397 47.250 124.128 1.00 43.98	O

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ATOM	284 CB LEU A 349	2.597 46.340 126.878 1.00 44.61	С
ATOM	285 CG LEU A 349		C
		1.354 48.294 125.964 1.00 45.55	С
		2.014 48.325 128.358 1.00 45.19	С
		5.489 45.958 125.615 1.00 43.72	N
<b>ATOM</b>	289 CA ALA A 350	6.818 46.432 125.216 1.00 42.64	С
ATOM	290 C ALA A 350	7.023 46.190 123.724 1.00 42.80	C
<b>ATOM</b>		7.291 47.135 122.996 1.00 42.61	0
<b>ATOM</b>	292 CB ALA A 350	7.949 45.739 125.956 1.00 41.26	С
ATOM	293 N ASP A 351		N
ATOM		6.997 44.638 121.871 1.00 45.42	C
ATOM			С
_		6.686 45.967 119.856 1.00 46.01	0
		6.633 43.184 121.612 1.00 47.72	C
ATOM	298 CG ASP A 351	6.905 42.840 120.149 1.00 50.33	С
ATOM	299 OD1 ASP A 351	8.043 42.706 119.656 1.00 49.95 5.887 42.687 119.433 1.00 53.18	0
ATOM		5.018 45.967 121.331 1.00 45.40	N
ATOM		4.237 46.886 120.529 1.00 45.67	
ATOM	303 C ARG A 352		C O
	304 U ARG A 332	4.937 48.907 119.502 1.00 47.67 2.817 46.836 121.056 1.00 46.38	C
ATOM	305 CB ARG A 352	2.174 45.538 120.584 1.00 48.04	C
		0.680 45.902 120.387 1.00 50.42	
		0.095 45.703 121.723 1.00 52.44	
		-0.723 46.610 122.289 1.00 53.34	
ATOM	310 NH1 ARG A 352	-1.042 47.739 121.644 1.00 52.42	N
		-1.132 46.217 123.500 1.00 53.07	N
		5.141 48.837 121.745 1.00 45.01	N
		5.680 50.194 121.773 1.00 43.53	С
		6.968 50.299 120.966 1.00 42.80	С
ATOM	315 O GLU A 353	7.305 51.370 120.459 1.00 43.00	0
ATOM	316 CB GLU A 353	5.966 50.620 123.198 1.00 43.41	C
ATOM	317 CG GLU A 353	4.910 50.245 124.204 1.00 44.09	C
ATOM	318 CD GLU A 353	5.154 50.924 125.538 1.00 44.78	С
ATOM	319 OE1 GLU A 353	5.187 52.154 125.617 1.00 43.92	0
ATOM	320 OE2 GLU A 353	5.323 50.176 126.525 1.00 46.56	0
ATOM	321 N LEU A 354	7.704 49.198 120.834 1.00 41.84	N
ATOM	322 CA LEU A 354	8.969 49.195 120.124 1.00 42.17	C
ATOM	323 C LEU A 354	8.804 49.655 118.698 1.00 42.86	<b>C</b> .
ATOM	324 O LEU A 354	9.616 50.399 118.160 1.00 42.54	0
ATOM	325 CB LEU A 354	9.642 47.827 120.218 1.00 41.39	C
ATOM	326 CG LEU A 354	10.467 47.775 121.518 1.00 41.35	C
ATOM	327 CD1 LEU A 354	10.648 46.351 121.978 1.00 41.91	C
ATOM	328 CD2 LEU A 354	11.783 48.483 121.295 1.00 41.15	C

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ATOM	329 N VAL A 355	7.698 49.203 118.103 1.00 43.57	N
		7.424 49.649 116.733 1.00 42.80	
ATOM	331 C VAL A 355	7.268 51.167 116.754 1.00 44.35	С
<b>ATOM</b>	332 O VAL A 355	7.982 51.901 116.058 1.00 44.80	Ο
		6.142 48.974 116.268 1.00 40.41	С
		5.838 49.431 114.878 1.00 39.85	С
ATOM	335 CG2 VAL A 355	6.385 47.492 116.364 1.00 41.41	С
		6.361 51.672 117.597 1.00 44.18	N
		6.178 53.115 117.631 1.00 45.93	C
ATOM	338 C HIS A 356	7.484 53.818 117.909 1.00 44.50	C
ATOM	340 CD LTC 4 356	7.691 54.886 117.348 1.00 44.30 5.074 53.470 118.667 1.00 49.34	0
			C C
ATOM	341 CO HIS A 330	3.801 52.906 118.115 1.00 51.75 2.806 53.687 117.571 1.00 53.41	N
ATOM	343 CD2 HIS A 356	3.422 51.617 117.985 1.00 52.93	
ATOM	344 CE1 HIS A 356	1.840 52.884 117.133 1.00 54.25	
ATOM	345 NE2 HIS A 356	2.186 51 619 117 369 1.00 54.33	N
ATOM	346 N MET A 357	8.303 53.240 118.784 1.00 43.74	N
ATOM	347 CA MET A 357	9.564 53.819 119.185 1.00 43.00	С
		10.472 54.177 118.015 1.00 42.86	
		10.973 55.288 117.903 1.00 42.82	
ATOM	350 CB MET A 357	10.385 52.909 120.117 1.00 42.65	С
ATOM	351 CG MET A 357	11.501 53.799 120.720 1.00 43.39 12.579 52.768 121.725 1.00 44.21	С
ATOM	352 SD MET A 357	12.579 52.768 121.725 1.00 44.21	<u>S</u> .
		11.526 52.625 123.168 1.00 44.48	. C
		10.665 53.188 117.151 1.00 42.08	N
ATOM	355 CA ILE A 358	11.465 53.306 115.961 1.00 40.73	C
ATOM	356 C ILE A 358	10.980 54.507 115.168 1.00 42.35	C
		11.811 55.315 114.760 1.00 43.21 11.334 52.029 115.114 1.00 39.01	O C
		11.888 50.851 115.908 1.00 38.76	
		12.064 52.170 113.799 1.00 37.79	=
	361 CD1 ILE A 358	11.865 49.519 115.206 1.00 38.39	Č
	362 N ASN A 359	9.683 54.631 114.950 1.00 44.26	N
	363 CA ASN A 359	9.114 55.742 114.220 1.00 46.79	С
ATOM	364 C ASN A 359	9.443 57.060 114.880 1.00 46.25	C · ·
<b>ATOM</b>	365 O ASN A 359	9.899 58.021 114.275 1.00 48.11	0
ATOM	366 CB ASN A 359	7.587 55.634 114.159 1.00 51.74	С
<b>ATOM</b>	367 CG ASN A 359	7.290 54.604 113.091 1.00 56.17	С
ATOM	368 OD1 ASN A 359	7.650 54.927 111.954 1.00 60.30	0
ATOM	369 ND2 ASN A 359	6.727 53.450 113.387 1.00 57.83	N
ATOM	370 N TRP A 360	9.230 57.118 116.178 1.00 44.87	N
ATOM		9.519 58.318 116.939 1.00 43.49	C
ATOM	372 C TRP A 360	10.969 58.707 116.765 1.00 43.83	С
ATOM	373 O TRP A 360	11.335 59.846 116.544 1.00 44.37	0

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***	70,50012	119/371	
ATOM	374 CB TRP A 360	9.268 57.954 118.392 1.00 42.53	С
ATOM	375 CG TRP A 360	9.913 58.953 119.301 1.00 43.10	С
ATOM	376 CD1 TRP A 360	9.463 60.210 119.571 1.00 43.10	C
ATOM	377 CD2 TRP A 360	11.114 58.770 120.057 1.00 43.07	C
ATOM	378 NE1 TRP A 360	10.314 60.817 120.448 1.00 43.67	N
ATOM	379 CE2 TRP A 360	11.335 59.958 120.768 1.00 43.61 12.019 57.723 120.194 1.00 43.09	C C
ATOM	380 CE3 TRP A 360 381 CZ2 TRP A 360	12.426 60.150 121.617 1.00 43.58	Č
ATOM ATOM	382 CZ3 TRP A 360	13.102 57.920 121.024 1.00 44.07	č
ATOM	383 CH2 TRP A 360	13.304 59.111 121.732 1.00 43.80	Č
ATOM	384 N ALA A 361	11.869 57.735 116.888 1.00 45.32	N
ATOM	385 CA ALA A 361	13.303 57.983 116.771 1.00 45.58	С
ATOM	386 C ALA A 361	13.575 58.748 115.489 1.00 46.83	С
ATOM	387 O ALA A 361	14.330 59.719 115.538 1.00 46.98	0
ATOM	388 CB ALA A 361	14.078 56.686 116.840 1.00 44.50	С
ATOM	389 N LYS A 362	12.959 58.380 114.372 1.00 48.34	N
ATOM		13.207 59.033 113.106 1.00 50.58	C C
ATOM ATOM	391 C LYS A 362 392 O LYS A 362	12.907 60.508 113.100 1.00 50.88 13.456 61.175 112.231 1.00 51.42	0
ATOM	393 CB LYS A 362	12.485 58.322 111.966 1.00 52.62	C
ATOM	394 CG LYS A 362		Č
ATOM	395 CD LYS A 362		Č
ATOM	396 CE LYS A 362	14.524 56.032 109.926 1.00 62.25	C
ATOM	397 NZ LYS A 362	15.709 56.341 109.035 1.00 64.54	N
ATOM	398 N ARG A 363	12.110 61.048 113.974 1.00 51.58	N
ATOM	399 CA ARG A 363	11.785 62.450 114.045 1.00 53.69	C
ATOM	400 C ARG A 363	12.594 63.209 115.090 1.00 53.02	С
ATOM	401 O ARG A 363 402 CB ARG A 363	12.305 64.399 115.299 1.00 <b>53</b> .79 10.315 62.631 114.474 1.00 <b>56</b> .98	O C
ATOM ATOM	402 CB ARG A 363 403 CG ARG A 363	9.582 61.312 114.322 1.00 63.56	Č
ATOM	404 CD ARG A 363	9.117 61.289 112.835 1.00 69.94	Č
ATOM		8.089 62.353 112.824 1.00 75.38	N
ATOM	406 CZ ARG A 363		С
ATOM	407 NH1 ARG A 363	6.676 61.046 114.134 1.00 79.67	N
ATOM	408 NH2 ARG A 363	6.051 63.193 113.446 1.00 80.13	N
ATOM	409 N VAL A 364	13.507 62.599 115.836 1.00 51.20	N
ATOM	410 CA VAL A 364	14.219 63.406 116.858 1.00 48.91	С
ATOM	411 C VAL A 364	15.256 64.176 116.076 1.00 48.54	C O
ATOM ATOM	412 O VAL A 364 413 CB VAL A 364	16.138 63.589 115.462 1.00 49.24 14.821 62.482 117.916 1.00 47.40	c
ATOM	414 CG1 VAL A 364	15.741 63.200 118.872 1.00 46.24	C
ATOM	415 CG2 VAL A 364	13.677 61.813 118.654 1.00 47.03	Č
ATOM		15.170 65.480 116.033 1.00 48.39	N
ATOM		16.097 66.322 115.282 1.00 47.91	С
ATOM	418 C PRO A 365	17.509 65.821 115.405 1.00 47.69	С

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ATOM	419 O PRO A 365	17.971 65.570 116.509 1.00 49.38	0
ATOM	420 CB PRO A 365	15.903 67.748 115.822 1.00 47.32	С
ATOM	421 CG PRO A 365	14.412 67.652 116.118 1.00 48.06	С
ATOM	422 CD PRO A 365	14.140 66.277 116.716 1.00 48.28	С
<b>ATOM</b>	423 N GLY A 366	18.197 65.616 114.304 1.00 47.73	N
<b>ATOM</b>	424 CA GLY A 366	19.573 65.178 114.242 1.00 47.06	С
<b>ATOM</b>	425 C GLY A 366	19.776 63.692 114.099 1.00 47.16	С
<b>ATOM</b>	426 O GLY A 366	20.835 63.259 113.659 1.00 47.88	О
<b>ATOM</b>	427 N PHE A 367	18.790 62.889 114.477 1.00 47.22	N
<b>ATOM</b>		18.889 61.440 114.464 1.00 47.22	С
ATOM	429 C PHE A 367	19.212 60.827 113.111 1.00 47.24	C
ATOM	430 () PHE A 367	20.124 60.047 112.830 1.00 46.44	0
ATOM		17.594 60.806 114.968 1.00 46.00	C C
ATOM		17.697 59.321 115.172 1.00 46.50	C
ATOM		18.426 58.795 116.232 1.00 46.47	C
ATOM		17.067 58.441 114.309 1.00 46.08 18.523 57.432 116.438 1.00 46.01	C
ATOM		17.160 57.074 114.528 1.00 46.50	c
ATOM	437 CZ PHE A 367		Č
ATOM ATOM	438 N VAL A 368		N
ATOM		18.374 60.858 110.797 1.00 47.41	Ċ
ATOM	440 C VAL A 368		c
ATOM		19.901 60.612 109.101 1.00 48.36	Ö
ATOM		17.125 61.454 110.136 1.00 46.86	C.
ATOM	443 CG1 VAL A 368	17,420 62.152 108.846 1.00 47.96	С
ATOM	444 CG2 VAL A 368	16.101 60.354 109.960 1.00 46.89	С
<b>ATOM</b>	445 N ASP A 369	20.424 62.189 110.616 1.00 48.68	N
<b>ATOM</b>	446 CA ASP A 369	21.695 62.531 110.013 1.00 49.52	С
<b>ATOM</b>	447 C ASP A 369		C
ATOM		23.787 61.548 109.748 1.00 49.03	0
ATOM		22.277 63.845 110.556 1.00 53.35	C
ATOM	450 CG ASP A 369		С
ATOM	451 OD1 ASP A 369	20.601 65.118 109.393 1.00 59.66	0
ATOM	452 OD2 ASP A 369	21.303 65.885 111.327 1.00 59.04	0
ATOM	453 N LEU A 370	22.522 60.450 111.138 1.00 46.30	N C
ATOM	454 CA LEU A 370	23.536 59.428 111.403 1.00 45.24 23.457 58.314 110.382 1.00 44.34	C
ATOM	455 C LEU A 370	22.434 58.171 109.701 1.00 43.23	Ö
ATOM	456 O LEU A 370	23,300 58.888 112.819 1.00 45.60	C
ATOM ATOM	457 CB LEU A 370 458 CG LEU A 370	23.446 59.923 113.939 1.00 45.74	c
ATOM	459 CD1 LEU A 370	23.173 59.313 115.301 1.00 45.87	C
ATOM	460 CD2 LEU A 370	24.871 60.487 113.901 1.00 45.51	C
ATOM	461 N THR A 371	24.499 57.499 110.215 1.00 44.24	N
ATOM	462 CA THR A 371	24.364 56.429 109.204 1.00 43.33	Ċ
ATOM	463 C THR A 371	23.278 55.478 109.682 1.00 44.46	C
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ATOM	464 O THR A 371	23.058 55.270 110.884 1.00 44.89	О
<b>ATOM</b>	465 CB THR A 371	25.644 55.614 109.113 1.00 42.88	С
<b>ATOM</b>	466 OG1 THR A 371	25.991 55.295 110.475 1.00 44.81	0
<b>ATOM</b>	467 CG2 THR A 371	26.725 56.466 108.523 1.00 43.53	С
<b>ATOM</b>	468 N LEU A 372		N
<b>ATOM</b>	469 CA LEU A 372		С
<b>ATOM</b>	470 C LEU A 372		C
<b>ATOM</b>	471 O LEU A 372	21.196 52.643 111.048 1.00 47.02	0
<b>ATOM</b>		21.134 53.178 107.795 1.00 42.97	C
<b>ATOM</b>	473 CG LEU A 372	20.398 54.060 106.787 1.00 41.97	C
<b>ATOM</b>	474 CD1 LEU A 372	20.048 53.301 105.517 1.00 42.70	C
		19.081 54.519 107.349 1.00 42.33	С
		23.218 52.342 110.147 1.00 46.19	N
		23.573 51.402 111.202 1.00 46.22	С
	478 C HIS A 373	23.685 52.125 112.517 1.00 45.75	C
ATOM		23.243 51.528 113.511 1.00 44.61	0
ATOM		24.830 50.649 110.770 1.00 49.78	C
ATOM	481 CG HIS A 373	24.489 49.599 109.749 1.00 52.88	C
ATOM		24.700 49.707 108.383 1.00 53.25	N
ATOM		23.924 48.383 109.900 1.00 53.27	C C
	484 CEI HIS A 373	24.281 48.599 107.798 1.00 53.55	N N
		23.789 47.764 108.710 1.00 53.71	N N
	486 N ASP A 374		C
ATOM		24.295 54.063 113.820 1.00 45.24	c
ATOM	488 C ASP A 374		0
ATOM	489 O ASP A 374	22.795 54.190 115.673 1.00 44.65 25.127 55.336 113.680 1.00 46.38	C
ATOM		26.554 54.825 113.562 1.00 49.02	C
ATOM		26.732 53.613 113.888 1.00 49.79	o
ATOM	492 OD1 ASE A 374	27.470 55.582 113.162 1.00 51.05	Ö
ATOM	493 UD2 ASF A 3/4	21.917 54.575 113.648 1.00 42.92	N
ATOM ATOM	495 CA GLN A 375	20.588 54.739 114.188 1.00 42.51	C
ATOM	496 C GLN A 375	20.207 53.417 114.817 1.00 43.01	C
ATOM	497 O GLN A 375	19.822 53.394 115.992 1.00 44.65	Ō
ATOM	498 CB GLN A 375	19.654 55.118 113.076 1.00 43.53	C
ATOM	499 CG GLN A 375	20.088 56.418 112.420 1.00 45.48	С
ATOM	500 CD GLN A 375	19.210 56.773 111.235 1.00 46.42	С
ATOM	501 OE1 GLN A 375	18.039 56.404 111.105 1.00 46.13	O
ATOM	502 NE2 GLN A 375	19.821 57.519 110.324 1.00 47.37	N
ATOM	503 N VAL A 376	20.329 52.291 114.126 1.00 42.62	N
ATOM	504 CA VAL A 376	19.983 51.018 114.772 1.00 42.53	С
ATOM	505 C VAL A 376	20.786 50.895 116.073 1.00 43.65	С
ATOM	506 O VAL A 376	20.260 50.529 117.143 1.00 44.09	Ο
ATOM	507 CB VAL A 376	20.187 49.810 113.862 1.00 41.72	С
ATOM	508 CG1 VAL A 376		С

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0

21.374 50.643 123.006 1.00 46.93

20.382 51.205 123.988 1.00 44.14

20.441 50.771 125.131 1.00 43.47

**ATOM** 

**ATOM** 

**ATOM** 

551 CA CYS A 381

552 C CYS A 381

553 O CYS A 381

·wo	98/56812	1	PCT/GB98/
		123/371	
ATOM	554 CB CYS A 381	22.630 51.531 122.807 1.00 52.10	С
ATOM	555 SG CYS A 381	24.154 50.637 123.375 1.00 64.30	S
ATOM		19.496 52.118 123.659 1.00 42.34	N
ATOM		18.576 52.724 124.604 1.00 40.77	C
ATOM		17.128 52.295 124.647 1.00 41.16	C
ATOM		16.307 52.896 125.364 1.00 41.74	0
ATOM		18.551 54.208 124.158 1.00 39.48	C
ATOM		16.712 51.243 123.952 1.00 40.69	N C
ATOM		15.292 50.882 123.935 1.00 39.18 14.642 50.806 125.292 1.00 38.59	C
ATOM	563 C TRP A 383 564 O TRP A 383	13.687 51.543 125.573 1.00 37.35	o
ATOM ATOM		15.150 49.646 123.083 1.00 38.87	C
ATOM		15.591 48.367 123.697 1.00 38.06	Č
ATOM		16.809 47.778 123.640 1.00 37.73	C
ATOM		14.746 47.501 124.465 1.00 37.97	Č
ATOM	569 NE1 TRP A 383	16.788 46.590 124.331 1.00 37.21	N
ATOM	570 CE2 TRP A 383	15.537 46.405 124.849 1.00 37.91	С
	571 CE3 TRP A 383	13.407 47.566 124.859 1.00 38.26	С
ATOM		15.018 45.371 125.622 1.00 38.84	С
ATOM		12.902 46.537 125.625 1.00 38.87	
ATOM		13.700 45.447 126.002 1.00 39.04	С
ATOM			N
ATOM		14.611 49.807 127.505 1.00 36.09	C
ATOM		14.721 51.083 128.318 1.00 35.10	C O
ATOM		13.826 51.348 129.112 1.00 34.48	C
ATOM		15.207 48.608 128.203 1.00 34.99 14.603 48.237 129.546 1.00 35.42	C
ATOM ATOM		13.092 48.090 129.521 1.00 35.66	C
ATOM		15.192 46.892 129.981 1.00 36.23	Č
ATOM		15.757 51.891 128.156 1.00 35.48	N
ATOM		15.848 53.129 128.939 1.00 36.88	С
ATOM		14.644 53.984 128.520 1.00 36.73	С
<b>ATOM</b>	586 O GLU A 385	13.861 54.383 129.411 1.00 35.40	Ο
<b>ATOM</b>	587 CB GLU A 385	17.181 53.836 128.798 1.00 38.31	С
ATOM	588 CG GLU A 385	18.326 53.543 129.749 1.00 38.88	С
ATOM	589 CD GLU A 385		C
ATOM	590 OE1 GLU A 385	20.219 53.786 128.322 1.00 40.13	0
ATOM	591 OE2 GLU A 385	20.062 55.285 129.931 1.00 42.21	0
ATOM	592 N ILE A 386	14.496 54.204 127.200 1.00 36.32	N
ATOM	593 CA ILE A 386	13.369 54.952 126.667 1.00 36.91	C
ATOM	594 C ILE A 386	12.015 54.392 127.175 1.00 37.34	C O .
ATOM	595 O ILE A 386	11.196 55.155 127.686 1.00 36.16 13.197 54.938 125.148 1.00 37.89	C
ATOM ATOM	596 CB ILE A 386 597 CG1 ILE A 386	14.449 55.123 124.299 1.00 39.71	C
ATOM	598 CG2 ILE A 386	12.193 56.015 124.799 1.00 37.70	Č
AIOM	376 CG2 ILL: A 380	12.175 50.015 127.777 1.00 57.70	•

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ATOM	599 CD1 ILE A 386	15.189 56.418 124.439 1.00 40.45	С
ATOM	600 N LEU A 387	11.763 53.082 127.072 1.00 37.39	N
ATOM	601 CA LEU A 387	10.544 52.515 127.573 1.00 37.91	С
ATOM	602 C LEU A 387	10.387 52.805 129.064 1.00 39.68	С
ATOM	603 O LEU A 387	9.240 53.071 129.463 1.00 41.71	O
ATOM	604 CB LEU A 387	10.494 50.992 127.494 1.00 38.33	С
ATOM	605 CG LEU A 387	10.120 50.317 126.176 1.00 38.87	С
ATOM	606 CD1 LEU A 387	10.162 48.800 126.371 1.00 37.89	С
ATOM	607 CD2 LEU A 387	8.789 50.804 125.606 1.00 37.40	С
ATOM	608 N MET A 388	11.476 52.739 129.858 1.00 39.41	N
ATOM	609 CA MET A 388	11.300 52.973 131.289 1.00 38.29	С
ATOM	610 C MET A 388	11.054 54.431 131.585 1.00 38.40	С
ATOM	611 O MET A 388	10.187 54.682 132.426 1.00 37.90	0
ATOM	612 CB MET A 388	12.409 52.456 132.178 1.00 38.21	C
ATOM	613 CG MET A 388	12.865 51.030 131.946 1.00 39.18	С
ATOM	614 SD MET A 388	13.843 50.384 133.298 1.00 41.37	S
ATOM	615 CE MET A 388	13.780 48.630 133.153 1.00 40.82	С
ATOM	616 N ILE A 389	11.731 55.378 130.921 1.00 39.23	N
ATOM		11.393 56.773 131.338 1.00 40.38	С
ATOM	618 C ILE A 389	9.953 57.105 130.980 1.00 41.61	С
ATOM	619 O ILE A 389	9.260 57.885 131.621 1.00 42.10	О
ATOM	620 CB ILE A 389	12.414 57.774 130.800 1.00 39.04	С
ATOM		12.194 59.163 131.402 1.00 38.47	С
ATOM	622 CG2 ILE A 389		С
ATOM	623 CD1 ILE A 389	13.371 60.102 131.204 1.00 37.35	С
ATOM	624 N GLY A 390	9.417 56.498 129.930 1.00 42.82	N
ATOM	625 CA GLY A 390	8.039 56.715 129.508 1.00 44.08	С
ATOM	626 C GLY A 390	7.109 56.228 130.618 1.00 44.05	C
ATOM	627 O GLY A 390	6.226 56.959 131.077 1.00 44.56	0
ATOM	628 N LEU A 391	7.356 54.992 131.035 1.00 42.62	N
ATOM	629 CA LEU A 391	6.511 54.453 132.100 1.00 42.62	C
ATOM	630 C LEU A 391		C
ATOM	631 O LEU A 391		0
ATOM	632 CB LEU A 391	7.071 53.088 132.498 1.00 42.08	C
ATOM	633 CG LEU A 391	6.485 52.463 133.747 1.00 42.23	C
ATOM	634 CD1 LEU A 391	4.983 52.285 133.530 1.00 43.26	C
ATOM	635 CD2 LEU A 391	7.126 51.127 134.055 1.00 42.49	C
ATOM	636 N VAL A 392	7.704 55.731 133.759 1.00 43.68	N
ATOM	637 CA VAL A 392	7.917 56.545 134.931 1.00 43.90	C
ATOM	638 C VAL A 392	7.100 57.813 134.814 1.00 44.98	С
ATOM	639 O VAL A 392	6.380 58.241 135.708 1.00 45.64	0
ATOM	640 CB VAL A 392	9.422 56.833 135.146 1.00 42.28	C C
ATOM	641 CG1 VAL A 392	9.675 57.920 136.172 1.00 42.44	C
ATOM	642 CG2 VAL A 392	10.088 55.603 135.729 1.00 42.06	
ATOM	643 N TRP A 393	7.242 58.436 133.664 1.00 46.50	N

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ATOM	644 CA TRP A 393	6.584 59.706 133.374 1.00 48.60	С
ATOM	645 C TRP A 393	5.073 59.618 133.392 1.00 49.25	С
ATOM	646 O TRP A 393	4.442 60.477 133.999 1.00 51.00	Ο
ATOM	647 CB TRP A 393	7.008 60.174 131.992 1.00 48.98	С
ATOM	648 CG TRP A 393	6.086 61.190 131.410 1.00 49.25	С
ATOM	649 CD1 TRP A 393	5.226 61.001 130.378 1.00 49.40	С
ATOM	650 CD2 TRP A 393	5.922 62.542 131.826 1.00 49.62	С
ATOM	651 NE1 TRP A 393	4.555 62.170 130.112 1.00 49.05	N
ATOM	652 CE2 TRP A 393	4.964 63.130 130.982 1.00 48.79	С
ATOM	653 CE3 TRP A 393	6.510 63.321 132.824 1.00 50.99	С
ATOM	654 CZ2 TRP A 393	4.580 64.458 131.090 1.00 48.79	С
ATOM	655 CZ3 TRP A 393	6.109 64.656 132.937 1.00 51.01	С
ATOM	656 CH2 TRP A 393	5.160 65.207 132.070 1.00 49.61	С
ATOM	657 N ARG A 394	4.524 58.609 132.717 1.00 49.10	N
ATOM	658 CA ARG A 394	3.079 58.463 132.729 1.00 48.80	С
<b>ATOM</b>	659 C ARG A 394	2.639 57.914 134.078 1.00 50.57	С
ATOM	660 O ARG A 394	1.430 57.901 134.332 1.00 53.43	Ο
ATOM	661 CB ARG A 394	2.483 57.616 131.634 1.00 47.23	С
ATOM	662 CG ARG A 394	3.134 56.353 131.161 1.00 46.71	С
<b>ATOM</b>	663 CD ARG A 394	2.386 55.724 129.994 1.00 45.21	С
ATOM	664 NE ARG A 394	2.758 54.304 129.908 1.00 45.92	N
ATOM	665 CZ ARG A 394	3.880 53.877 129.315 1.00 45.48	С
ATOM	666 NH1 ARG A 394	4.639 54.850 128.808 1.00 45.47	N
ATOM	667 NH2 ARG A 394	4.192 52.585 129.253 1.00 43.51	N
ATOM	668 N SER A 395	3.506 57.457 134.959 1.00 51.48	N
ATOM	669 CA SER A 395	3.096 56.916 136.243 1.00 52.31	С
ATOM	670 C SER A 395	3.171 57.963 137.341 1.00 54.06	C
ATOM	671 O SER A 395		0
ATOM	672 CB SER A 395		C
ATOM		3.659 54.564 136.024 1.00 49.71	0
ATOM	674 N MET A 396	3.621 59.161 136.995 1.00 56.81	N
ATOM	675 CA MET A 396	3.791 60.223 137.959 1.00 60.16	C
ATOM	676 C MET A 396	2.654 60.519 138.925 1.00 63.28	C
ATOM	677 O MET A 396	2.823 60.538 140.153 1.00 63.48	0
ATOM	678 CB MET A 396	4.030 61.519 137.188 1.00 59.66	C
ATOM	679 CG MET A 396	5.202 62.300 137.761 1.00 60.46	C
ATOM	680 SD MET A 396	5.832 63.284 136.390 1.00 63.79	S C
ATOM	681 CE MET A 396	5.681 64.939 137.052 1.00 63.38	N
ATOM	682 N GLU A 397	1.464 60.775 138.386 1.00 66.02	C
ATOM	683 CA GLU A 397	0.324 61.111 139.209 1.00 69.12	C
ATOM	684 C GLU A 397	-0.378 59.904 139.747 1.00 67.67	
ATOM	685 O GLU A 397	-1.597 59.964 139.945 1.00 68.94 -0.737 61.932 138.471 1.00 74.43	O C
ATOM	686 CB GLU A 397		C
ATOM	687 CG GLU A 397	-0.192 63.107 137.671 1.00 80.96	C
ATOM	688 CD GLU A 397	0.439 62.557 136.400 1.00 85.44	C

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ATOM	689 OE1 GLU A 397		0
ATOM	690 OE2 GLU A 397	1.293 63.251 135.796 1.00 88.68	0
<b>ATOM</b>	691 N HIS A 398	0.215 58.755 139.964 1.00 65.64	N
<b>ATOM</b>	692 CA HIS A 398	-0.448 57.589 140.514 1.00 64.64	С
ATOM	693 C HIS A 398	0.563 57.044 141.525 1.00 63.33	С
<b>ATOM</b>	694 O HIS A 398	1.182 56.010 141.286 1.00 64.30	0
ATOM	695 CB HIS A 398	-0.808 56.503 139.512 1.00 65.95	С
ATOM	696 CG HIS A 398	-1.800 56.931 138.480 1.00 67.89	С
ATOM	697 ND1 HIS A 398	-1.581 58.093 137.754 1.00 68.76	N
<b>ATOM</b>	698 CD2 HIS A 398	-2.970 56.441 138.015 1.00 68.33	С
ATOM	699 CE1 HIS A 398	-2.553 58.322 136.904 1.00 68.97	С
ATOM	700 NE2 HIS A 398	-3.408 57.317 137.047 1.00 69.03	N
ATOM	701 N PRO A 399	0.738 57.788 142.593 1.00 60.98	N
ATOM	702 CA PRO A 399	1.678 57.460 143.639 1.00 60.04	С
<b>ATOM</b>	703 C PRO A 399	1.573 56.008 144.013 1.00 58.72	С
<b>ATOM</b>	704 O PRO A 399	0.479 55.479 144.144 1.00 60.15	0
<b>ATOM</b>	705 CB PRO A 399	1.307 58.333 144.857 1.00 60.42	С
ATOM	706 CG PRO A 399	0.722 59.525 144.140 1.00 60.58	С
<b>ATOM</b>	707 CD PRO A 399	0.029 59.010 142.914 1.00 60.38	С
ATOM	708 N GLY A 400	2.676 55.323 144.127 1.00 57.37	N
ATOM	709 CA GLY A 400	2.658 53.933 144.519 1.00 57.37	С
<b>ATOM</b>	710 C GLY A 400	2.241 52.954 143.467 1.00 56.93	С
<b>ATOM</b>	711 O GLY A 400	2.226 51.744 143.762 1.00 57.91	О
ATOM	712 N LYS A 401	1.931 53.447 142.279 1.00 56.53	N
ATOM	713 CA LYS A 401	1,508 52,589 141,185 1.00 56,36	С
ATOM	714 C LYS A 401	2.264 52.906 139.886 1.00 54.56	С
ATOM	715 O LYS A 401	2.864 53.977 139.700 1.00 53.14	0
ATOM	716 CB LYS A 401	0.041 52.772 140.841 1.00 58.66	C
ATOM	717 CG LYS A 401	-0.982 52.903 141.935 1.00 61.77	C
ATOM	718 CD LYS A 401	-1.890 51.680 141.909 1.00 65.18	С
ATOM	719 CE LYS A 401	-2.620 51.475 143.237 1.00 66.98	С
ATOM	720 NZ LYS A 401	-3.156 52.790 143.712 1.00 69.54	N
ATOM	721 N LEU A 402	2.172 51.896 139.007 1.00 51.98	N
ATOM	722 CA LEU A 402	2.813 52.052 137.708 1.00 50.19	C
ATOM	723 C LEU A 402	1.734 51.837 136.656 1.00 49.79	C
ATOM	724 O LEU A 402	1.148 50.766 136.579 1.00 50.90	0
ATOM	725 CB LEU A 402	3.972 51.108 137.434 1.00 49.03	C
ATOM	726 CG LEU A 402	5.170 51.118 138.369 1.00 48.58	C
ATOM	727 CD1 LEU A 402	5.995 49.842 138.211 1.00 49.67	C
ATOM	728 CD2 LEU A 402	6.035 52.333 138.144 1.00 46.96	C
ATOM	729 N LEU A 403	1.485 52.844 135.859 1.00 48.94	N
ATOM	730 CA LEU A 403	0.560 52.836 134.755 1.00 48.00	С
ATOM	731 C LEU A 403	1.171 52.346 133.445 1.00 48.26	C
ATOM	732 O LEU A 403	1.502 53.141 132.540 1.00 46.38	0
ATOM	733 CB LEU A 403	0.157 54.309 134.499 1.00 49.14	С

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		127/371	
ATOM	734 CG LEU A 403	-1.143 54.414 133.705 1.00 50.00	С
<b>ATOM</b>	735 CD1 LEU A 403	-2.347 54.243 134.616 1.00 51.26	С
<b>ATOM</b>	736 CD2 LEU A 403	-1.218 55.729 132.979 1.00 50.69	С
ATOM	737 N PHE A 404	1.320 51.014 133.299 1.00 48.71	N
ATOM	738 CA PHE A 404		С
ATOM	739 C PHE A 404	1.035 51.013 130.872 1.00 49.94	C
ATOM	740 O PHE A 404	1.593 51.449 129.875 1.00 50.84	0
ATOM	741 CB PHE A 404	1.939 48.961 131.983 1.00 48.34	C
ATOM	742 CG PHE A 404		С
ATOM		2.917 48.338 134.176 1.00 49.16	C
ATOM		4.381 48.409 132.309 1.00 48.46	С
ATOM		3.989 47.974 134.994 1.00 48.97	C
ATOM	· · · · <del>· - · · · · · · · · · · · · · ·</del>	5.438 48.054 133.130 1.00 48.15	C
ATOM	747 CZ PHE A 404	5.245 47.831 134.468 1.00 47.67	C
ATOM	748 N ALA A 405	-0.277 50.939 131.000 1.00 51.36	N C
ATOM		-1.254 51.416 130.046 1.00 52.93	C
ATOM	750 C ALA A 405	-2.365 52.175 130.749 1.00 54.33	Ö
ATOM	751 O ALA A 405	-2.547 52.092 131.967 1.00 56.08 -1.856 50.215 129.350 1.00 53.05	C
ATOM	752 CB ALA A 405 753 N PRO A 406	-3.219 52.850 129.995 1.00 54.64	N
ATOM		-4.366 53.602 130.483 1.00 54.88	C
ATOM ATOM	755 C PRO A 406	-5.275 52.556 131.109 1.00 55.66	c
ATOM	756 O PRO A 406	-5.948 52.873 132.087 1.00 58.90	o
ATOM	757 CB PRO A 406	-5.037 54.376 129.367 1.00 53.81	C
ATOM		-4.033 54.176 128.275 1.00 54.41	č
ATOM		-3.182 52.956 128.551 1.00 54.81	Ċ
ATOM	760 N ASN A 407	-5.250 51.347 130.590 1.00 54.42	N
ATOM	761 CA ASN A 407	-6.030 50.281 131.148 1.00 54.72	С
ATOM	762 C ASN A 407	-5.158 49.201 131.762 1.00 55.68	С
ATOM	763 O ASN A 407	-5.566 48.020 131.772 1.00 56.97	0
ATOM	764 CB ASN A 407	-6.924 49.703 130.059 1.00 55.56	С
ATOM	765 CG ASN A 407	-6.093 48.843 129.120 1.00 55.68	С
ATOM	766 OD1 ASN A 407	-4.958 49.154 128.814 1.00 56.47	0
ATOM	767 ND2 ASN A 407	-6.631 47.739 128.670 1.00 56.02	N
ATOM	768 N LEU A 408	-3.970 49.522 132.274 1.00 55.43	N
ATOM	769 CA LEU A 408	-3.196 48.472 132.980 1.00 54.67	С
ATOM	770 C LEU A 408	-2.441 49.270 134.032 1.00 54.84	C
ATOM	771 O LEU A 408	-1.520 49.964 133.660 1.00 54.42	0_
ATOM	772 CB LEU A 408	-2.282 47.623 132.172 1.00 55.04	C
ATOM	773 CG LEU A 408	-1.389 46.584 132.848 1.00 54.56	C
ATOM	<del>_</del>	-2.143 45.735 133.845 1.00 53.43	C
ATOM		-0.746 45.703 131.772 1.00 54.04	C
ATOM	776 N LEU A 409	-2.920 49.190 135.268 1.00 55.99	N
ATOM	777 CA LEU A 409	-2.287 49.971 136.344 1.00 55.11	С
ATOM	778 C LEU A 409	-1.816 49.041 137.434 1.00 55.12	С

128/371 -2.616 48.795 138.321 1.00 57.05 O **ATOM** 779 O LEU A 409 C -3.328 50.959 136.781 1.00 54.28 **ATOM** 780 CB LEU A 409 C **ATOM** 781 CG LEU A 409 -3.147 51.968 137.874 1.00 55.28 C -1.724 52.458 138.053 1.00 56.18 782 CD1 LEU A 409 ATOM 783 CD2 LEU A 409 -3.999 53.209 137.569 1.00 55.71 C **ATOM** N -0.608 48.499 137.370 1.00 55.36 ATOM 784 N LEU A 410 -0.172 47.598 138.422 1.00 56.40 C **ATOM** 785 CA LEU A 410 C 0.221 48.429 139.634 1.00 58.86 ATOM 786 C LEU A 410 0.460 49.643 139.561 1.00 59.46 O 787 O LEU A 410 ATOM C 788 CB LEU A 410 0.933 46.656 137.991 1.00 54.82 ATOM 789 CG LEU A 410 C 0.558 45.942 136.687 1.00 54.21 ATOM 790 CD1 LEU A 410 1.681 45.031 136.207 1.00 54.45 C **ATOM** 791 CD2 LEU A 410 C -0.733 45.192 136.922 1.00 53.26 ATOM 792 N ASP A 411 0.223 47.704 140.730 1.00 60.91 N **ATOM** 0.543 48.300 142.026 1.00 64.05 C 793 CA ASP A 411 ATOM 1.813 47.646 142.525 1.00 63.96 C 794 C ASP A 411 ATOM 795 O ASP A 411 2.061 46.481 142.172 1.00 63.71 0 **ATOM** 796 CB ASP A 411 -0.721 48.022 142.835 1.00 68.11 C **ATOM** -0.415 47.770 144.298 1.00 71.79 C 797 CG ASP A 411 ATOM 798 OD1 ASP A 411 0.217 46,705 144,523 1.00 73.88 0 ATOM -0.793 48.646 145.116 1.00 73.30 799 OD2 ASP A 411 0 ATOM 800 N ARG A 412 2.612 48.326 143.354 1.00 64.12 N ATOM 3.862 47.709 143.787 1.00 64.43 C 801 CA ARG A 412 ATOM 3.761 46.216 144.061 1.00 65.36 C ATOM 802 C ARG A 412 4.413 45.368 143.449 1.00 65.53 0 ATOM 803 O ARG A 412 4.473 48.394 144.996 1.00 63.99 C 804 CB ARG A 412 ATOM C ATOM 805 CG ARG A 412 5.476 47.466 145.681 1.00 64.51 6.364 48,216 146,642 1.00 65.90 C 806 CD ARG A 412 ATOM 7.612 47.514 146.947 1.00 66.08 807 NE ARG A 412 N ATOM 7.631 46.359 147.595 1.00 66.60 C 808 CZ ARG A 412 ATOM 809 NH1 ARG A 412 6,489 45,798 147,977 1.00 66.50 N ATOM 8.794 45.782 147.852 1.00 67.25 N ATOM \$10 NH2 ARG A 412 2.936 45.816 145.001 1.00 66.84 N 811 N ASN A 413 ATOM 2.798 44.419 145.363 1.00 69.21 C 812 CA ASN A 413 ATOM 813 C ASN A 413 2.524 43.498 144.218 1.00 69.03 C ATOM 2.983 42.348 144.280 1.00 69.61 0 814 O ASN A 413 ATOM C 815 CB ASN A 413 1.703 44.331 146.438 1.00 73.12 ATOM \$16 CG ASN A 413 2.124 45.327 147.524 1.00 76.06 C ATOM 0 817 OD1 ASN A 413 3.078 44.994 148.239 1.00 77.88 ATOM 818 ND2 ASN A 413 1.452 46.472 147.569 1.00 76.66 N ATOM 1.883 43.910 143.128 1.00 68.31 N 819 N GLN A 414 ATOM 320 CA GLN A 414 1.642 43.008 141.997 1.00 67.98 C ATOM C \$21 C GLN A 414 2.953 42.619 141.323 1.00 67.67 ATOM 3.059 41.664 140.555 1.00 67.18 0 S22 O GLN A 414 ATOM \$23 CB GLN A 414 0.647 43.591 141.021 1.00 68.30 C ATOM

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ATOM	869 C MET A 421	10.198 43,267 140.603 1.00 60.86	С
ATOM	870 O MET A 421	10.126 44.429 140.222 1.00 61.61	0
ATOM	871 CB MET A 421	9.053 41.763 139.110 1.00 63.01	С
	872 CG MET A 421	9.155 41.484 137.618 1.00 64.57	С
ATOM	873 SD MET A 421	8.600 42.941 136.721 1.00 65.96	S
ATOM	874 CE MET A 421	6.843 42.583 136.658 1.00 65.26	С
ATOM	875 N VAL A 422	9.991 42.978 141.865 1.00 59.84	N
ATOM	876 CA VAL A 422	9.671 43.990 142.842 1.00 59.34	С
<b>ATOM</b>	877 C VAL A 422	10.763 45.031 142.941 1.00 58.27	С
ATOM	878 O VAL A 422	10.400 46.177 143.150 1.00 58.27	O
<b>ATOM</b>	879 CB VAL A 422	9.513 43.477 144.290 1.00 60.52	С
<b>ATOM</b>	880 CG1 VAL A 422	8.283 44.098 144.911 1.00 59.97	С
<b>ATOM</b>	881 CG2 VAL A 422	8.283 44.098 144.911 1.00 59.97 9.511 41.954 144.331 1.00 62.39	С
<b>ATOM</b>	882 N GLUA 423	12.014 44.624 142.845 1.00 57.88	N
<b>ATOM</b>		13.093 45.582 143.002 1.00 58.53	С
ATOM	884 C GLU A 423	13.054 46.565 141.842 1.00 56.03	С
ATOM	885 O GLU A 423	13.268 47.771 142.015 1.00 56.14	0
ATOM	886 CB GLU A 423	14.465 44.939 143.057 1.00 63.31	С
ATOM	887 CG GLU A 423	14.635 43.901 144.141 1.00 69.88	C
ATOM		14.211 42.522 143.622 1.00 74.05	C
ATOM	889 OE1 GLU A 423	12.986 42.214 143.553 1.00 74.81	0
		15.172 41.762 143.287 1.00 76.76	0
ATOM		12.801 45.987 140.672 1.00 52.17	N C
ATOM		12.714 46.851 139.483 1.00 49.13 11.538 47.787 139.678 1.00 48.36	C
ATOM		11.673 49.013 139.527 1.00 48.89	Ö
ATOM ATOM		12.648 45.948 138.262 1.00 48.08	C
ATOM		13.983 45.195 138.186 1.00 47.42	C
ATOM		12.405 46.751 137.013 1.00 48.16	Č
ATOM		13.943 44.144 137.105 1.00 47.58	Č
ATOM		10.384 47.274 140.097 1.00 46.94	N
ATOM	900 CA PHE A 425	9.231 48.116 140.345 1.00 47.55	С
ATOM	901 C PHE A 425	9.587 49.199 141.354 1.00 49.35	С
ATOM	902 O PHE A 425	9.195 50.366 141.213 1.00 49.71	Ο
<b>ATOM</b>	903 CB PHE A 425	8.081 47.277 140.882 1.00 47.68	C
<b>ATOM</b>	904 CG PHE A 425	7.176 46.715 139.829 1.00 48.82	C
ATOM	905 CD1 PHE A 425	7.680 46.377 138.573 1.00 49.52	С
ATOM	906 CD2 PHE A 425	5.825 46.514 140.070 1.00 48.28	С
ATOM	907 CE1 PHE A 425	6.899 45.863 137.561 1.00 48.30	C
ATOM	908 CE2 PHE A 425	5.038 45.994 139.058 1.00 49.20	С
ATOM	909 CZ PHE A 425	5.557 45.670 137.808 1.00 48.67	C
ATOM	910 N ASP A 426	10.341 48.806 142.386 1.00 50.36	N
ATOM	911 CA ASP A 426	10.737 49.750 143.426 1.00 50.81	C
ATOM	912 C ASP A 426	11.527 50.902 142.852 1.00 50.50	C
ATOM	913 O ASP A 426	11.176 52.085 143.041 1.00 49.63	0

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ATOM	914 CB ASP A 426	11.406 48.954 144.534 1.00 53.65	С
ATOM	915 CG ASP A 426	10.316 48.430 145.473 1.00 56.55	Ċ
ATOM	916 OD1 ASP A 426	9.170 48.940 145.384 1.00 57.43	Ō
ATOM	917 OD2 ASP A 426	10.590 47.529 146.301 1.00 58.16	O
ATOM	918 N MET A 427	12.575 50.575 142.083 1.00 49.66	N
ATOM	919 CA MET A 427	13.396 51.606 141.438 1.00 47.62	C
ATOM	920 C MET A 427	12.538 52.483 140.529 1.00 46.03	c
ATOM	921 O MET A 427	12.679 53.726 140.504 1.00 44.60	Ö
ATOM	922 CB MET A 427	14.476 50.885 140.655 1.00 48.02	C
ATOM	923 CG MET A 427	15.467 50.239 141.617 1.00 49.42	Č
ATOM	924 SD MET A 427	16.870 49.639 140.649 1.00 51.75	S
ATOM	925 CE MET A 427	16.149 48.109 140.031 1.00 50.74	Č
ATOM	926 N LEU A 428	11.627 51.786 139.817 1.00 43.62	N
ATOM	927 CA LEU A 428	10.719 52.557 138.954 1.00 43.05	С
ATOM	928 C LEU A 428	9.879 53,529 139.779 1.00 43.69	С
ATOM	929 O LEU A 428	9.804 54.738 139.487 1.00 43.73	0
ATOM	930 CB LEU A 428	9.884 51.598 138.134 1.00 41.42	С
ATOM	931 CG LEU A 428	10.630 50.884 137.008 1.00 39.99	С
ATOM	932 CD1 LEU A 428	9.754 49.788 136.444 1.00 39.57	C
ATOM	933 CD2 LEU A 428	11.004 51.865 135.920 1.00 40.09	С
ATOM	934 N LEU A 429	9.262 53.032 140.866 1.00 43.31	N
ATOM	935 CA LEU A 429	8.457 53.947 141.688 1.00 42.48	С
ATOM	936 C LEU A 429	9.273 55.104 142.224 1.00 42.48	С
ATOM	937 O LEU A 429	8.897 56.281 142.110 1.00 42.82	0
ATOM	938 CB LEU A 429	7.725 53.158 142.761 1.00 41.76	С
ATOM	939 CG LEU A 429	6.674 52.197 142.202 1.00 41.28	С
ATOM	940 CD1 LEU A 429	6.320 51.130 143.211 1.00 42.51	С
ATOM	941 CD2 LEU A 429	5.404 52.920 141.801 1.00 41.15	С
ATOM	942 N ALA A 430	10.452 54.808 142.769 1.00 42.41	N
ATOM	943 CA ALA A 430	11.304 55.886 143.268 1.00 42.66	С
ATOM	944 C ALA A 430	11.554 56.960 142.217 1.00 43.57	С
ATOM	945 O ALA A 430	11.573 58.158 142.539 1.00 44.26	0
ATOM	946 CB ALA A 430	12.642 55.300 143.679 1.00 41.40	C
ATOM	947 N THR A 431	11.794 56.562 140.959 1.00 43.33	N
ATOM	948 CA THR A 431	12.075 57.589 139.956 1.00 44.07	С
ATOM	949 C THR A 431	10.814 58.382 139.711 1.00 45.04	C
ATOM	950 O THR A 431	10.793 59.607 139.615 1.00 45.47	0
ATOM	951 CB THR A 431	12.460 56.942 138.612 1.00 45.00	C
ATOM	952 OG1 THR A 431	13.421 55.921 138.929 1.00 46.49	0
ATOM	953 CG2 THR A 431	12.973 57.967 137.624 1.00 43.41	C
ATOM	954 N SER A 432	9.724 57.606 139.612 1.00 46.10	N
ATOM	955 CA SER A 432	8.414 58.218 139.367 1.00 47.08	С
	956 C SER A 432	8.124 59.288 140.409 1.00 46.69	C
	957 O SER A 432	7.747 60.409 140.153 1.00 45.78	0
ATOM	958 CB SER A 432	7.350 57.120 139.344 1.00 47.86	С

997 NH1 ARG A 436

998 NH2 ARG A 436

999 N MET A 437

1000 CA MET A 437

1002 O MET A 437

ATOM 1001 C MET A 437

ATOM 1003 CB MET A 437

4.389 60.109 143,224 1.00 72.66

4.939 60.419 144.399 1.00 72.98

4.428 58.850 142.770 1.00 72.97

8.708 65.953 143.586 1.00 69.37

8.157 64.942 142.711 1.00 66.55

9.295 67.133 142.836 1.00 68.28

9.152 68.261 143.317 1.00 69.47

9.815 65.340 144.427 1.00 75.02

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ATOM	1049 CG GLU A 443	7.530 72.149 127.143 1.00 65.79	С
ATOM	1050 CD GLU A 443	6.392 71.931 128.137 1.00 68.13	С
		6.621 71.911 129.369 1.00 68.25	
ATOM	1052 OE2 GLU A 443	5.256 71.763 127.630 1.00 69.95	0
ATOM	1053 N GLU A 444	10.101 69.205 129.445 1.00 53.20	N
		11.331 68.677 130.012 1.00 51.24	
		11.397 67.171 129.727 1.00 50.05	
		12.444 66.683 129.258 1.00 50.87 11.372 68.890 131.514 1.00 50.94	
ATOM	1057 CB GLUA 444	11.572 08.890 131.314 1.00 30.94	C
ATOM	1059 CD GLU A 444	11.608 70.359 131.856 1.00 51.30 11.499 70.564 133.365 1.00 51.90	č
ATOM	1060 OE1 GLU A 444	10.606 69.965 134.020 1.00 51.11	O
		12.349 71.353 133.839 1.00 52.20	
<b>ATOM</b>	1062 N PHE A 445	10.282 66.481 129.989 1.00 46.38	N
ATOM	1063 CA PHE A 445	10.254 65.055 129.738 1.00 44.95	C
ATOM	1064 C PHE A 445	10.728 64.714 128.336 1.00 45.48	С
		11.613 63.901 128.118 1.00 47.22	
ATOM	1066 CB PHE A 445	8.844 64.523 129.927 1.00 43.54	C
ATOM	1067 CG PHE A 445	8.615 63.149 129.369 1.00 43.00 9.314 62.082 129.885 1.00 43.66	С
ATOM	1068 CD1 PHE A 445	9.314 62.082 129.885 1.00 43.66	C
ATOM	1009 CD2 PHE A 445	7.726 62.898 128.353 1.00 42.85 9.132 60.799 129.421 1.00 44.24	C C
		7.502 61.627 127.874 1.00 43.01	
ATOM	1072 CZ PHE A 445	8 207 60 574 128 415 1 00 44 06	C
ATOM	1073 N VAL A 446	8.207 60.574 128.415 1.00 44.06 10.158 65.315 127.329 1.00 45.92	N
ATOM	1074 CA VAL A 446	10.458 65.099 125.919 1.00 46.59	С
		11.915 65.347 125.625 1.00 48.14	
		12.579 64.661 124.811 1.00 49.23	
ATOM	1077 CB VAL A 446	9.400 65.935 125.178 1.00 46.86	C
ATOM	1078 CG1 VAL A 446	9.928 66.958 124.216 1.00 46.55 8.437 64.956 124.504 1.00 47.00	С
ATOM	1079 CG2 VAL A 446	8.437 64.956 124.504 1.00 47.00	
	1081 CA CYS A 447	12.545 66.323 126.279 1.00 48.23	N C
	1082 C CYS A 447	13.965 66.562 126.046 1.00 48.88 14.829 65.451 126.609 1.00 48.68	c
	1083 O CYS A 447	15.747 64.958 125.966 1.00 49.55	O
	1084 CB CYS A 447	14.346 67.868 126.761 1.00 50.37	C
	1085 SG CYS A 447	13.962 69.266 125.693 1.00 54.72	Š
	1086 N LEU A 448	14.573 65.046 127.857 1.00 47.78	N
ATOM	1087 CA LEU A 448	15.344 63.993 128.499 1.00 46.35	С
	1088 C LEU A 448	15.277 62.710 127.679 1.00 46.10	С
	1089 O LEU A 448	16.301 62.054 127.425 1.00 47.12	O
	1090 CB LEU A 448	14.819 63.712 129.882 1.00 47.13	C
	1091 CG LEU A 448	15.095 64.717 130.993 1.00 48.03	C
ATOM	1092 CD1 LEU A 448		C
AIUM	1093 CD2 LEU A 448	16.577 64.837 131.306 1.00 47.62	С

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		20,109 63,428 120,129 1.00 44.81	C
	1140 CD2 LEU A 454		C
	1141 N ASN A 455	22.533 59.909 123.869 1.00 45.07	N
	1142 CA ASN A 455	23.768 59.745 124.627 1.00 45.73	С
	1143 C ASN A 455	24.057 58.330 125.013 1.00 48.44	C
ATOM	1144 O ASN A 455		0
ATOM	1145 CB ASN A 455		C
ATOM	1146 CG ASN A 455	24.714 60.421 126.940 1.00 45.06	С
		24.312 59.878 127.981 1.00 46.01	O N
	1148 ND2 ASN A 455	25.991 60.781 126.797 1.00 45.17	N
ATOM		23.085 57.454 125.143 1.00 51.91	C
ATOM	1150 CA SER A 456	23.403 56.111 125.615 1.00 54.70 24.368 55.318 124.791 1.00 57.99	c
ATOM	1151 C SER A 456 1152 O SER A 456		0
ATOM	1152 O SER A 456		C
	1154 OG SER A 456		Ö
	1155 N GLY A 457		N
-	1156 CA GLY A 457		C
ATOM	1157 C GLY A 457		C
ATOM	1158 O GLY A 457		O
ATOM	1159 N VAL A 458		N
ATOM	1160 CA VAL A 458		С
ATOM	i 161 C VAL A 458		С
ATOM	1162 O VAL A 458		0
	1163 CB VAL A 458		C
	1164 CG1 VAL A 458		C
	1165 CG2 VAL A 458		C
	1166 N TYR A 459		N
		30.674 55.650 123.410 1.00 84.10	C C
	1168 C TYR A 459 1169 O TYR A 459		Ö
	1170 CB TYR A 459	4	Ċ
ATOM	1170 CB TYR A 459		Č
	1172 CD1 TYR A 459		C
	1173 CD2 TYR A 459		C
	1174 CE1 TYR A 459		C
	1175 CE2 TYR A 459		С
	1176 CZ TYR A 459		С
	1177 OH TYR A 459		0
	1178 N THR A 460	30.044 53.813 121.918 1.00 89.04	N
ATOM	1179 CA THR A 460		С
ATOM		29.764 52.501 119.880 1.00 92.95	C
ATOM		29.011 51.660 119.381 1.00 93.70	0
ATOM			C
ATOM	1183 OG1 THR A 46	28.435 52.146 123.118 1.00 92.33	Ο

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ATOM	1184	CG2 THR A 460	30.036 50.433 122.802 1.00 93.11	С
<b>ATOM</b>	1185	N PHE A 461	30.293 53.485 119.156 1.00 94.66	N
ATOM	1186	CA PHE A 461	29.937 53.571 117.743 1.00 95.99	С
ATOM	1187	C PHE A 461	30.457 52.502 116.795 1.00 97.27	C
ATOM	1188	O PHE A 461	29.707 52.075 115.884 1.00 97.97	0
ATOM	1189	CB PHE A 461	30.195 55.012 117.234 1.00 95.00	С
ATOM	1190	CG PHE A 461	28.849 55.690 117.222 1.00 93.86	С
ATOM	1191	CD1 PHE A 461	27.708 54.934 117.036 1.00 93.38	С
ATOM	1192	CD2 PHE A 461	28.725 57.045 117.407 1.00 94.19	С
ATOM	1193	CE1 PHE A 461	26.467 55.505 117.024 1.00 93.79	С
ATOM	1194	CE2 PHE A 461	27.478 57.635 117.393 1.00 94.10	С
ATOM	1195	CZ PHE A 461	26.349 56.866 117.199 1.00 94.05	С
<b>ATOM</b>	1196	N THR A 465	35.765 54.719 111.803 1.00128.15	N
ATOM	1197	CA THR A 465	36.448 55.536 112.810 1.00128.00	С
ATOM	1198	C THR A 465	36.314 57.024 112.518 1.00126.85	С
ATOM	1199	O THR A 465	35.594 57.732 113.235 1.00127.19	О
<b>ATOM</b>	1200	CB THR A 465	37.934 55.169 112.971 1.00128.63	С
ATOM	1201	OG1 THR A 465	38.671 56.294 113.484 1.00128.85	O
ATOM	1202	CG2 THR A 465	38.536 54.747 111.634 1.00128.96	С
ATOM	1203	N LEU A 466	36.948 57.527 111.457 1.00124.68	N
<b>ATOM</b>	1204	CA LEU A 466	36.834 58.946 111.109 1.00 <b>122.3</b> 6	С
ATOM	.1205	C LEU A 466	35.380 59.372 110.897 1.00120.14	С
ATOM	1206	O LEU A 466	35.004 60.513 111.209 1.00120.35	0
ATOM	1207	CB LEU A 466		С
ATOM	1211	N LYS A 467	34.533 58.469 110.392 1.00116.55	N
ATOM		CA LYS A 467	33.110 58.730 110.232 1.00112.66	С
ATOM		C LYS A 467	32.523 58.682 111.649 1.00108.51	C
ATOM		O LYS A 467	31.602 59.430 111.937 1.00108.43	0
ATOM		CB LYS A 467		C
ATOM		CG LYS A 467	_	C
ATOM		CD LYS A 467		C
		CE LYS A 467		C
ATOM	1219	NZ LYS A 467	29.774 55.614 106.152 1.00117.07	N
ATOM		N SER A 468	33.064 57.846 112.522 1.00103.37	N
ATOM		CA SER A 468	32.609 57.753 113.889 1.00 99.63	C
ATOM		C SER A 468	32.923 59.038 114.652 1.00 96.39	C
ATOM		O SER A 468	32.132 59.534 115.442 1.00 95.91	0
ATOM		CB SER A 468	33.292 56.622 114.662 1.00100.41	C
ATOM		OG SER A 468	32.848 55.358 114.205 1.00101.46	0
ATOM		N LEU A 469	34.110 59.577 114.391 1.00 92.71	N
ATOM		CA LEU A 469	34.540 60.806 115.050 1.00 89.37	C
ATOM		C LEU A 469	33.583 61.906 114.627 1.00 86.96	С
ATOM	1229		33.213 62.769 115.417 1.00 86.78	0
ATOM		CB LEU A 469	36.009 61.096 114.755 1.00 89.59	C
ATOM	1234	N GLU A 470	33.150 61.868 113.379 1.00 84.76	N

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ATOM	1235 CA GLU A 470	32.201 62.860 112.869 1.00 83.39	С
ATOM	1236 C GLU A 470	30.812 62.559 113.408 1.00 79.41	C
	1237 O GLU A 470		0
ATOM	1238 CB GLU A 470	32.342 62.911 111.369 1.00 87.27	C
		31.065 62.883 110.562 1.00 92.97	C
		31.323 62.549 109.097 1.00 96.39	С
		32.446 62.061 108.788 1.00 98.06	0
	1242 OE2 GLU A 470		0
	1243 N GLU A 471 1244 CA GLU A 471		N C
	1245 C GLU A 471		c
		28.128 61.791 116.075 1.00 70.94	Ö
ATOM	1247 CB GLU A 471	28.981 59.375 113.974 1.00 69.61	c
ATOM	1248 CG GLU A 471	28.789 58.802 112.604 1.00 68.52	C
ATOM	1249 CD GLU A 471	27.388 58.530 112.148 1.00 68.47	C
<b>ATOM</b>	1250 OE1 GLU A 471	26.700 57.643 112.673 1.00 68.63	0
		26.838 59.174 111.232 1.00 68.52	О
	1252 N LYS A 472		N
	1253 CA LYS A 472	30.304 61.470 117.680 1.00 67.78	C
	1254 C LYS A 472		C
	1255 O LYS A 472		0
		31.582 61.016 118.375 1.00 69.03 31.596 59.526 118.666 1.00 71.43	C C
ATOM	1257 CO LTS A 472	32.719 59.148 119.613 1.00 74.06	C ·
		33.355 57.803 119.260 1.00 76.26	Č
		32.614 56.637 119.848 1.00 77.74	N
	1261 N ASP A 473		N
	1262 CA ASP A 473	30.640 65.221 117.111 1.00 65.40	С
ATOM	1263 C ASP A 473	29.199 65.672 116.927 1.00 62.92	С
		28.600 66.391 117.720 1.00 63.45	O
		31.424 66.063 116.113 1.00 69.21	C
	1266 CG ASP A 473	32.907 65.839 116.318 1.00 73.72	C
	1267 OD1 ASP A 473	33.269 65.168 117.325 1.00 76.19	0
	1268 OD2 ASP A 473 1269 N HIS A 474	33.656 66.347 115.447 1.00 75.94 28.641 65.217 115.819 1.00 59.42	O N
	1270 CA HIS A 474	27,262 65.532 115.494 1.00 55.77	C
	1271 C HIS A 474	26.393 65.294 116.722 1.00 54.86	c
	1272 O HIS A 474	25.647 66.153 117.187 1.00 53.76	Ö
	1273 CB HIS A 4 <b>7</b> 4	26.866 64.629 114.329 1.00 54.89	C
	1274 CG HIS A 474	25.458 65.016 113.979 1.00 55.54	C
	1275 ND1 HIS A 474	25.171 66.330 113.614 1.00 55.25	N
ATOM	1276 CD2 HIS A 474	24.313 64.286 113.980 1.00 55.43	С
ATOM	1277 CE1 HIS A 474	23.866 66.361 113.387 1.00 56.29	С
	1278 NE2 HIS A 474	23.320 65.149 113.598 1.00 55.98	N
ATOM	1279 N ILE A 475	26.480 64.088 117.288 1.00 54.45	N

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ATOM	1325		23.049 71.538 123.043 1.00 52.02	С
ATOM	1326	O ASP A 480	22.474 72.234 123.894 1.00 52.76	0
			25.530 71.463 122.818 1.00 52.27	С
ATOM	1328	CG ASP A 480	26.854 70.920 123.300 1.00 53.57	С
<b>ATOM</b>	1329	OD1 ASP A 480	26.911 70.289 124.371 1.00 54.43	0
			27.896 71.110 122.621 1.00 53.82	0
			22.555 71.404 121.820 1.00 53.08	N
			21.331 72.106 121.440 1.00 54.53	
		C LYS A 481		C
			19.568 72.572 122.972 1.00 54.44	0
			20.954 71.790 120.005 1.00 58.12	C
ATOM	1336	CG LYS A 481	19.876 72.721 119.466 1.00 63.38	C
ATOM	1337	CD LYS A 481	20.501 73.909 118.728 1.00 67.75	C
ATOM	1338	CE LYS A 481	19.617 75.156 118.745 1.00 70.46	C
			18.636 75.201 119.889 1.00 72.21 20.016 70.405 122.634 1.00 52.20	N N
			18.973 69.958 123.549 1.00 50.20	
			19.228 70.564 124.915 1.00 49.24	c
ATOM	1343	O ILE A 482	18.284 71.029 125.561 1.00 48.46	Ö
ATOM	1344	CB ILE A 482	18.795 68.444 123.582 1.00 49.95	C
ATOM	1345	CG1 ILE A 482	18.259 67.970 122.225 1.00 49.93	C
ATOM	1346	CG2 ILE A 482	17.788 67.989 124.619 1.00 49.78	
			18.887 66.663 121.792 1.00 49.98	
			20.476 70.622 125.344 1.00 49.25	
ATOM	1349	CA THR A 483	20.752 71.251 126.637 1.00 50.71	
		C THR A 483		С
			19.466 73.054 127.592 1.00 51.98	
			22.260 71.245 126.953 1.00 49.92	
ATOM	1353	OG1 THR A 483	22.590 69.868 127.144 1.00 48.98	
			22.564 72.031 128.221 1.00 50.19	C
		N ASP A 484	20.596 73.439 125.576 1.00 51.42 20.142 74.829 125.467 1.00 50.56	N C
ATOM ATOM		C ASP A 484	18.630 74.827 125.528 1.00 49.52	c
		O ASP A 484	18.030 74.897 125.328 1.00 45.32	0
		CB ASP A 484	20.661 75.526 124.233 1.00 51.89	C
		CG ASP A 484	22.179 75.649 124.176 1.00 53.29	C ·
		OD1 ASP A 484	22.841 75.588 125.240 1.00 53.06	0
		OD2 ASP A 484	22.706 75.807 123.039 1.00 53.68	0
		N THR A 485	17.958 74.020 124.804 1.00 49.22	N
		CA THR A 485	16.493 74.000 124.867 1.00 49.37	С
ATOM	1365	C THR A 485	16.010 73.836 126.288 1.00 50.25	С
		O THR A 485	15.052 74.495 126.664 1.00 51.49	0
		CB THR A 485	16.011 72.824 124.002 1.00 48.58	C
		OG1 THR A 485		0
ATOM	1369	CG2 THR A 485	14.507 72.817 123.930 1.00 47.80	С

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ATOM	1370 N LEU A 486	16.646 72.984 127.084 1.00 51.08	N
ATOM	1371 CA LEU A 486	16,235 72.755 128.462 1.00 50.84	С
ATOM	1372 C LEU A 486	16.336 74.020 129.300 1.00 51.72	С
ATOM	1373 O LEU A 486	15.392 74.395 130.004 1.00 50.51	Ο
ATOM	1374 CB LEU A 486	17.083 71.660 129.124 1.00 48.86	С
ATOM		16.471 70.263 129.060 1.00 47.10	Č
	1376 CD1 LEU A 486	17.415 69.268 129.691 1.00 45.88	C
	1377 CD2 LEU A 486	15.096 70.250 129.689 1.00 46.89	C
ATOM	1378 N ILE A 487	17.513 74.654 129.183 1.00 53.22	N
ATOM	1379 CA ILE A 487	17.705 75.893 129.962 1.00 55.44	C
ATOM	1380 C ILE A 487	16.687 76.950 129.526 1.00 57.52	C
ATOM	1381 O ILE A 487	16.035 77.649 130.299 1.00 57.79	Ö
ATOM		19.102 76.458 129.740 1.00 54.89	Č
ATOM	1383 CG1 ILE A 487	20.160 75.546 130.329 1.00 55.18	Č
ATOM	1384 CG2 ILE A 487	19.110 77.846 130.342 1.00 55.82	č
ATOM	1385 CD1 ILE A 487	20.418 75.650 131.804 1.00 54.44	č
ATOM	1386 N HIS A 488	16.531 77.063 128.204 1.00 59.32	N
	1387 CA HIS A 488	15.571 77.978 127.629 1.00 60.40	Ċ
ATOM	1388 C HIS A 488	14.232 77.757 128.321 1.00 59.31	c
ATOM	1389 O HIS A 488	13.649 78.686 128.844 1.00 60.16	ŏ
ATOM	1390 CB HIS A 488	15,408 77,680 126,142 1.00 63,58	C
ATOM	1391 CG HIS A 488	14.246 78.450 125.585 1.00 67.04	Č
ATOM		14.282 79.820 125.450 1.00 68.39	N
	1393 CD2 HIS A 488	13.025 78.034 125.163 1.00 68.41	c
ATOM	1394 CE1 HIS A 488	13.114 80.206 124.939 1.00 69.75	č
ATOM	1395 NE2 HIS A 488	12.335 79.151 124.751 1.00 69.52	N
ATOM	1396 N LEU A 489	13.736 76.538 128.329 1.00 58.27	N
	1397 CA LEU A 489	12.481 76.237 128.963 1.00 58.66	Ċ
	1398 C LEU A 489	12.402 76.732 130.400 1.00 59.58	c
ATOM	1399 O LEU A 489	11.403 77.276 130.854 1.00 59.17	Ö
ATOM		12.311 74.713 128.965 1.00 58.09	Č
ATOM	1401 CG LEU A 489		Č
	1402 CD1 LEU A 489	12.022 72.613 127.653 1.00 59.37	C
	1403 CD2 LEU A 489		Č
	1404 N MET A 490		N
	1405 CA MET A 490	13.534 76.844 132.581 1.00 62.01	C
	1406 C MET A 490	13.545 78.337 132.851 1.00 62.91	C
	1407 O MET A 490	12.912 78.802 133.806 1.00 64.21	Ö
	1408 CB MET A 490	14.828 76.267 133.171 1.00 62.02	C
	1409 CG MET A 490	14.631 74.896 133.800 1.00 62.27	Č
	1410 SD MET A 490	16.240 74.108 133.935 1.00 63.57	S
	1411 CE MET A 490	15.813 72.389 133.645 1.00 63.55	Č
		14.282 79.049 132.003 1.00 62.99	N
		14.346 80.503 132.143 1.00 63.54	C
	1414 C ALA A 491		c
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ATOM	1415	O ALA A 491	12.370 81.706 132.732 1.00 63.44	0
		CB ALA A 491	15,297 81,131 131,150 1,00 63,64	С
		N LYS A 492	12.293 80.539 130.827 1.00 64.75	N
ATOM	1418	CA LYS A 492	10.914 80.911 130.527 1.00 65.96	С
<b>ATOM</b>	1419	C LYS A 492	10.021 80.636 131.715 1.00 66.48	С
ATOM	1420	O LYS A 492	9.077 81.396 131.931 1.00 68.10	Ο
ATOM	1421	CB LYS A 492	10.378 80.274 129.245 1.00 66.21	С
ATOM		N ALA A 493	10.251 79.654 132.568 1.00 67.14	N
ATOM		CA ALA A 493	9.427 79.420 133.741 1.00 68.33	С
		C ALA A 493	9.936 80.330 134.867 1.00 69.79	С
		O ALA A 493	9.512 80.309 136.034 1.00 70.80	0
		CB ALA A 493	9.451 77.976 134.198 1.00 68.17	С
		N GLY A 494	10.904 81.171 134.533 1.00 70.02	N
		CA GLY A 494	11.503 82.121 135.424 1.00 70.56	С
		C GLY A 494	12.186 81.486 136.606 1.00 70.48	C
		O GLY A 494	11.743 81.753 137.723 1.00 71.77	0
		N LEU A 495	13.210 80.665 136.388 1.00 70.08	N
		CA LEU A 495	13.898 80.138 137.574 1.00 69.07	C
ATOM ATOM		C LEU A 495 O LEU A 495	15.184 80.965 137.611 1.00 69.25 15.641 81.270 136.500 1.00 69.64	C O
		CB LEU A 495	14.322 78.702 137.497 1.00 68.82	C
		CG LEU A 495	13.325 77.646 137.061 1.00 68.59	C
		CD1 LEU A 495	13.911 76.265 137.307 1.00 68.14	C
		CD2 LEU A 495	12.019 77.824 137.802 1.00 69.34	C
_		N THR A 496	15.704 81.275 138.775 1.00 69.48	N
		CA THR A 496	16.970 82.025 138.757 1.00 70.96	C
		C THR A 496	18.014 81.334 137.905 1.00 71.12	C
		O THR A 496	17.950 80.134 137.620 1.00 72.23	O
ATOM	1447	CB THR A 496	17.559 81.950 140.176 1.00 71.91	С
ATOM	1,448	OG1 THR A 496	16.519 82.393 141.074 1.00 73.47	0
		CG2 THR A 496	18.843 82.729 140.317 1.00 72.96	C
		N LEU A 497	19.065 82.027 137.519 1.00 71.69	N
		CA LEU A 497	20.155 81.450 136.753 1.00 72.39	С
		C LEU A 497	20.770 80.305 137.571 1.00 72.97	С
		O LEU A 497	21.251 79.298 137.030 1.00 73.58	0
		CB LEU A 497	21.204 82.515 136.508 1.00 73.26	C
		CG LEU A 497	21.841 82.644 135.139 1.00 74.83	C
		CD1 LEU A 497	23.368 82.634 135.296 1.00 74.97	C
		CD2 LEU A 497	21.349 81.612 134.139 1.00 75.25	C
		N GLN A 498	20.771 80.433 138.896 1.00 72.53	N
_		CA GLN A 498	21.320 79.378 139.727 1.00 72.61	C
		C GLN A 498	20.306 78.254 139.801 1.00 71.51	C
		O GLN A 498	20.710 77.090 139.784 1.00 72.93	0
ATOM		CB GLN A 498	21.699 79.865 141.117 1.00 75.13	C C
ATOM	1403	CG GLN A 498	21.645 78.783 142.173 1.00 78.79	C

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	1509 N ARG A 503	18.556 72.607 138.574 1.00 50.84	N
ATOM		17.570 71.742 137.948 1.00 49.11	С
		18.224 70.926 136.833 1.00 48.91	C
		18.000 69.712 136.750 1.00 51.21	0
	1513 CB ARG A 503	16.434 72.514 137.261 1.00 48.05	C
	1514 CG ARG A 503	15.201 71.634 137.089 1.00 46.69	С
	1515 CD ARG A 503	13.958 72.465 136.865 1.00 45.33	C
	1516 NE ARG A 503	12.869 71.641 136.368 1.00 46.09	N
	1517 CZ ARG A 503	11.992 70.959 137.112 1.00 46.32	C
		12.076 70.988 138.438 1.00 45.38	N
	1519 NH2 ARG A 503	11.022 70.243 136.533 1.00 45.97	N
	1520 N LEU A 504	19.020 71.592 136.000 1.00 46.31	N
	1521 CA LEU A 504	19.671 70.862 134.922 1.00 45.01	C
	1522 C LEU'A 504	20.351 69.636 135.509 1.00 45.72	С
	1523 O LEU A 504	20.031 68.494 135.196 1.00 46.55	0
	1524 CB LEU A 504	20.701 71.708 134.184 1.00 42.72	C
	1525 CG LEU A 504	21.245 71.069 132.910 1.00 41.21	С
	1526 CD1 LEU A 504 1527 CD2 LEU A 504	20.175 70.645 131.929 1.00 39.03 22.269 72.018 132.296 1.00 41.69	C C
	1528 N ALA A 505 1529 CA ALA A 505	21.284 69.921 136.418 1.00 46.05	N C
	1530 C ALA A 505	22.020 68.842 137.071 1.00 45.12 21.039 67.884 137.720 1.00 46.07	c
	1531 O ALA A 505	21.214 66.659 137.531 1.00 47.92	0
		23.023 69.450 138.011 1.00 47.92	C
	1533 N GLN A 506	19.999 68.330 138.426 1.00 45.79	N
ATOM	1534 CA GLN A 506	19.110 67.322 139.006 1.00 47.26	C
ATOM	1535 C GLN A 506	18.472 66.448 137.940 1.00 47.55	c
	1536 O GLN A 506	18.349 65.234 138.187 1.00 48.38	Ö
		18.075 67.845 140.001 1.00 48.39	C
ATOM		18.389 69.172 140.639 0.50 50.04	C
ATOM	1539 CG BGLN A 506	18.778 68.216 141.328 0.50 47.76	Ċ
	1540 CD AGLN A 506	17.416 69.734 141.642 0.50 50.64	C
	1541 CD BGLN A 506	19.110 67.009 142.176 0.50 47.69	Č
	1542 OE1AGLN A 506		O
	1543 OE1BGLN A 506	18.592 65.912 141.895 0.50 48.97	0
	1544 NE2AGLN A 506		N
	1545 NE2BGLN A 506		N
ATOM	1546 N LEU A 507	18.084 67.008 136.804 1.00 47.58	N
<b>ATOM</b>	1547 CA LEU A 507	17.459 66.207 135.760 1.00 47.73	С
ATOM	1548 C LEU A 507	18.407 65.182 135.162 1.00 47.79	С
	1549 O LEU A 507	18.096 63.974 135.131 1.00 49.51	0
ATOM	1550 CB LEU A 507	16.882 67.108 134.685 1.00 48.50	С
	1551 CG LEU A 507	15.653 67.920 135.116 1.00 48.92	С
	1552 CD1 LEU A 507	15.253 68.828 133.952 1.00 50.13	С
ATOM	1553 CD2 LEU A 507	14.525 67.009 135.551 1.00 48.10	С

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				N
		N LEU A 508	19.567 65.615 134.707 1.00 46.56	N C
		CA LEU A 508	20.567 64.717 134.132 1.00 44.95 21.067 63.710 135.148 1.00 44.15	c
		C LEU A 508 O LEU A 508	21.378 62.581 134.708 1.00 45.36	O
ATOM		CB LEU A 508	21.720 65.557 133.551 1.00 44.88	C
		CG LEU A 508	21,283 66.552 132.472 1.00 44.46	C
		CD1 LEU A 508	22,431 67,354 131,935 1.00 44,78	c
		CD2 LEU A 508	20.679 65.822 131.280 1.00 46.15	č
		N LEU A 509	21.128 63.978 136.459 1.00 42.06	N
		CA LEU A 509	21.579 62.893 137.340 1.00 42.07	C
		C LEU A 509	20.557 61.753 137.417 1.00 42.29	C
		O LEU A 509	20.954 60.618 137.723 1.00 42.42	0
		CB LEU A 509	21.964 63.302 138.749 1.00 41.22	С
ATOM	1567	CG LEU A 509	23.239 64.117 138.912 1.00 40.99	С
ATOM	1568	CD1 LEU A 509	23.332 64.611 140.339 1.00 40.83	С
		CD2 LEU A 509		С
		N ILEA510	19.275 61.989 137.116 1.00 42.24	N
		CA ILE A 510	18.297 60.895 137.130 1.00 42.89	С
ATOM		C ILE A 510	18.639 59.913 136.004 1.00 41.94	C
ATOM		O ILE A 510	18.438 58.698 136.142 1.00 41.71	0
			16.841 61.359 137.037 1.00 42.87	C
			16.335 61.760 138.439 1.00 44.12	С
		<del></del> -	15.874 60.297 136.573 1.00 42.19	C
ATOM		CD1 ILE A 510	15.616 63.111 138.389 1.00 45.79	C N
		N LEU A 511	19.196 60.421 134.908 1.00 40.88 19.551 59.554 133.800 1.00 42.29	C
		CA LEU A 511 C LEU A 511		c
		O LEU A 511	20.372 57.273 133.739 1.00 43.47	Ö
			20.138 60.345 132.646 1.00 42.79	C
			19.232 61.427 132.042 1.00 42.59	Č
			19.905 61.905 130.754 1.00 42.80	Ċ
			17.832 60.894 131.792 1.00 41.41	С
		N SER A 512	21.353 58.661 135.190 1.00 42.45	N ·
		CA SER A 512	22.199 57.597 135.692 1.00 41.97	С
<b>ATOM</b>	1588	C SER A 512	21.372 56.441 136.243 1.00 41.74	С
		O SER A 512	21.593 55,272 135.918 1.00 41.94	0
		CB SER A 512	22.949 58.205 136.883 1.00 42.66	C
		OG SER A 512	24.235 57.651 136.722 1.00 46.60	0
		N HIS A 513	20.399 56.796 137.105 1.00 40.14	N
		CA HIS A 513	19.529 55.785 137.693 1.00 38.64	С
		C HIS A 513	18.762 55.039 136.606 1.00 39.44	С
		O HIS A 513	18.646 53.790 136.644 1.00 39.11	0
		CB HIS A 513	18.604 56.417 138.732 1.00 37.52	C
		CG AHIS A 513	19.490 56.911 139.845 0.50 38.84	C C
ATUM	1398	CG BHIS A 513	17.864 55.372 139.515 0.50 37.43	C

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		19.619 58.233 140.201 0.50 39.06	
ATOM	1600 ND1BHIS A 513	16.517 55.464 139.814 0.50 37.66	
ATOM	1601 CD2AHIS A 513	20.322 56.227 140.676 0.50 39.28	
		18.299 54.212 140.074 0.50 37.23	
	1603 CE1AHIS A 513		
ATOM	1604 CEIBHIS A 513	16.153 54.396 140.518 0.50 37.66	C
ATOM	1606 NE2ARIS A 513	20.919 57.143 141.514 0.50 38.49 17.217 53.622 140.689 0.50 37.60	N N
		18.281 55.782 135.589 1.00 38.07	N
		17.584 55.117 134.490 1.00 37.70	C
		18.533 54.140 133.822 1.00 37.71	c
ATOM	1610 O ILE A 514	18.163 52.987 133.547 1.00 37.51	Ō
		16.950 56.154 133.575 1.00 38.13	С
ATOM	1612 CG1 ILE A 514	15.716 56.726 134.296 1.00 37.64	С
		16.570 55.603 132.205 1.00 38.53	
ATOM	1614 CD1 ILE A 514	15.430 58.128 133.808 1.00 37.44	С
		19.796 54.505 133.622 1.00 38.16	
		20.745 53.542 133.034 1.00 39.24	
		20.775 52.305 133.936 1.00 39.63 20.592 51.168 133.503 1.00 39.61	
		22.162 54.093 132.921 1.00 39.22	C
		23.163 53.364 132.063 1.00 40.21	C
		22.636 53.155 130.689 1.00 44.06	
		23.587 53.120 129.576 1.00 46.91	
<b>ATOM</b>	1623 CZ ARG A 515	24.178 54.247 129.165 1.00 48.77	С
		23.949 55.429 129.752 1.00 49.82	N
	1625 NH2 ARG A 515		N
	1626 N HIS A 516		N
		21.081 51.538 136.221 1.00 38.90	С
		19.936 50.555 136.121 1.00 39.18 20.140 49.355 135.970 1.00 37.84	
		21.210 52.115 137.656 1.00 39.60	O C
	1631 CG HIS A 516	21.440 50.946 138.595 1.00 39.71	C
	1632 ND1 HIS A 516	22.613 50.238 138.674 1.00 39.57	N
	1633 CD2 HIS A 516	20.608 50.321 139.453 1.00 39.43	С
<b>ATOM</b>	1634 CE1 HIS A 516	22.520 49.253 139.520 1.00 38.56	С
	1635 NE2 HIS A 516	21.300 49.283 140.017 1.00 38.92	N
	1636 N MET A 517	18.707 51.044 136.207 1.00 41.07	N
	1637 CA MET A 517	17.480 50.261 136.129 1.00 41.63	С
	1638 C MET A 517	17.341 49.430 134.871 1.00 41.41	C
	1639 O MET A 517	16.945 48.280 134.891 1.00 40.72	0
	1640 CB MET A 517 1641 CG MET A 517	16.298 51.237 136.037 1.00 42.72	C C
	1642 SD MET A 517	15.515 51.311 137.335 1.00 44.29 14.274 52.640 137.213 1.00 45.43	S
	1643 CE MET A 517		S C
	OE WELLASIT	15.101 54.007 157.540 1.00 47.02	C

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ATOM	1644 N SER A 518	17.681 50.082 133.758 1.00 42.10	N
ATOM	1645 CA SER A 518	17.638 49.441 132.446 1.00 42.47	С
ATOM	1646 C SER A 518	18.569 48.244 132.411 1.00 42.00	С
ATOM	1647 O SER A 518	18.200 47.199 131.873 1.00 42.03	0
ATOM	1648 CB SER A 518	18.007 50.484 131.407 1.00 43.32	C
ATOM	1649 OG SER A 518	18.544 49.964 130.228 1.00 45.64	0
ATOM	1650 N ASN A 519	19.748 48.392 132.990 1.00 42.37	N
ATOM	1651 CA ASN A 519	20.713 47.295 133.030 1.00 44.29	С
ATOM	1652 C ASN A 519	20.084 46.169 133.831 1.00 44.94	С
ATOM	1653 O ASN A 519	20.079 45.036 133.362 1.00 46.19	0
ATOM	1654 CB ASN A 519	22.059 47.736 133.597 1.00 47.08	С
ATOM	1655 CG ASN A 519	22.911 48.548 132.631 1.00 49.35	С
ATOM	1656 OD1 ASN A 519	22.901 48.175 131.438 1.00 51.40	О
ATOM	1657 ND2 ASN A 519	23.625 49.607 133.033 1.00 48.18	N
ATOM	1658 N LYS A 520	19.498 46.414 134.995 1.00 44.94	N
ATOM	1659 CA LYS A 520	18.871 45.362 135.763 1.00 45.92	С
ATOM	1660 C LYS A 520	17.671 44.792 135.027 1.00 46.12	С
ATOM	1661 O LYS A 520		0
ATOM	1662 CB LYS A 520	18.367 45.898 137.088 1.00 48.44	С
ATOM	1663 CG LYS A 520	19.437 46.800 137.700 1.00 50.91	С
ATOM	1664 CD LYS A 520	20.181 45.926 138.689 1.00 53.34	С
ATOM	1665 CE LYS A 520	21.647 45.782 138.339 1.00 55.85	С
ATOM	1666 NZ LYS A 520	22.201 44.573 139.041 1.00 58.02	N
ATOM	1667 N GLY A 521	16.918 45.665 134.365 1.00 45.54	N
ATOM	1668 CA GLY A 521	15.807 45.181 133.568 1.00 45.58	С
ATOM	1669 C GLY A 521	16.270 44.202 132.482 1.00 45.78	C
ATOM	1670 O GLY A 521	15.561 43.182 132.432 1.00 45.24	0
ATOM	1671 N MET A 522	17.328 44.439 131.676 1.00 45.68	N
ATOM	1672 CA MET A 522	17.660 43.456 130.663 1.00 46.96	С
ATOM	1673 C MET A 522	18.061 42.141 131.346 1.00 48.31	C
ATOM	1674 O MET A 522	17.612 41.095 130.901 1.00 48.01	o
ATOM	1675 CB MET A 522		C
ATOM	1676 CG MET A 522	19.335 44.821 129.041 1.00 47.52	C
ATOM	1677 SD MET A 522	18.355 45.460 127.700 1.00 48.79	S
ATOM	1678 CE MET A 522	17.616 43.967 127.040 1.00 46.55	C
ATOM	1679 N GLU A 523	18.909 42.283 132.369 1.00 49.71	N
ATOM	1680 CA GLU A 523	19.336 41.083 133.075 1.00 51.07	С
ATOM	1681 C GLU A 523	18.137 40.248 133.475 1.00 48.53	C
ATOM	1682 O GLU A 523	18.134 39.039 133.310 1.00 48.65	0
ATOM	1683 CB GLU A 523	20.203 41.486 134.239 1.00 57.61	C
ATOM	1684 CG GLU A 523	21.688 41.593 133.956 1.00 64.95	C
ATOM	1685 CD GLU A 523	22.270 40.403 133.199 1.00 69.95	C
ATOM	1686 OE1 GLU A 523	21.645 39.297 133.221 1.00 72.64	0
ATOM	1687 OE2 GLU A 523	23.373 40.581 132.589 1.00 72.19	0
ATOM	1688 N HIS A 524	17.075 40.836 133.978 1.00 46.39	N

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ATOM	1689	CA HIS A 524	15.865 40.144 134.344 1.00 45.35	С
ATOM	1690	C HIS A 524	15.097 39.606 133.156 1.00 45.66	С
ATOM	1691	O HIS A 524	14.678 38.453 133.149 1.00 45.67	0
ATOM	1692	CB HIS A 524	14.953 41.109 135.115 1.00 43.98	С
ATOM	1693	CG HIS A 524	13.627 40.538 135.470 1.00 43.57	С
ATOM	1694	ND1 HIS A 524	12.542 40.552 134.611 1.00 44.22	N
ATOM	1695	CD2 HIS A 524	13.185 39.925 136.580 1.00 43.73	С
<b>ATOM</b>	1696	CE1 HIS A 524	11.505 39.982 135.189 1.00 44.25	С
ATOM	1697	NE2 HIS A 524	11.855 39.579 136.402 1.00 43.68	N
ATOM	1698	N LEU A 525	14.873 40.389 132.110 1.00 47.35	N
ATOM	1699	CA LEU A 525	14.074 39.974 130.954 1.00 49.08	С
<b>ATOM</b>	1700	C LEU A 525	14.721 38.741 130.341 1.00 51.79	С
ATOM	1701	O LEU A 525	14.098 37.840 129.819 1.00 51.57	Ο
ATOM	1702	CB LEU A 525	13.912 41.078 129.907 1.00 47.41	С
ATOM	1703	CG LEU A 525	13.259 40.641 128.599 1.00 46.29	C
ATOM	1704	CD1 LEU A 525	11.822 40.216 128.816 1.00 45.85	С
ATOM	1705	CD2 LEU A 525	13.321 41.793 127.618 1.00 45.98	С
ATOM	1706	N TYR A 526	16.043 38.747 130.444 1.00 55.42	N
ATOM	1707	CA TYR A 526	16.912 37.700 129.978 1.00 58.28	С
ATOM	1708	C TYR A 526	16.695 36.442 130.791 1.00 58.73	С
<b>ATOM</b>	1709	O TYR A 526	16.532 35.382 130.189 1.00 59.67	0
ATOM	1710	CB TYR A 526	18.351 38.203 130.088 1.00 60.44	С
ATOM	1711	CG TYR A 526	19.231 37.154 129.479 1.00 63.65	С
ATOM	1712	CD1 TYR A 526	19.396 37.063 128.120 1.00 66.19	C
			19.864 36.252 130.293 1.00 66.21	С
ATOM	1714	CE1 TYR A 526	20.206 36.096 127.562 1.00 69.05	С
ATOM	1715	CE2 TYR A 526	20.685 35.266 129.777 1.00 68.96	С
ATOM	1716	CZ TYR A 526	20.835 35.211 128.415 1.00 70.55	С
ATOM			21.647 34.235 127.874 1.00 74.44	Ο
			16.663 36.506 132.116 1.00 59.86	N
			16.424 35.244 132.848 1.00 61.25	С
			14.992 34.837 132.564 1.00 61.87	С
ATOM			14.818 33.689 132.186 1.00 62.52	0
_			16.686 35.314 134.336 1.00 61.10	C
		OG SER A 527	16.238 36.600 134.712 1.00 61.91	0
		N MET A 528	14.008 35.720 132.619 1.00 62.93	N
		CA MET A 528	12.643 35.385 132.249 1.00 63.77	С
		C MET A 528	12.615 34.640 130.920 1.00 64.50	C
ATOM	1727		11.878 33.669 130.756 1.00 63.77	0
ATOM		CB MET A 528	11.800 36.650 132.126 1.00 64.26	C
ATOM		CG MET A 528	11.182 37.186 133.395 1.00 64.61	C
		SD MET A 528	10.838 35.959 134.659 1.00 65.93	S
ATOM		CE MET A 528	12.311 36.036 135.659 1.00 64.66	С
ATOM		N LYS A 529	13.400 35.038 129.935 1.00 66.98	N
ATOM	1733	CA LYS A 529	13.464 34.355 128.651 1.00 70.45	С

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ATOM	1734 C	LYS A 529	14.098 32.973 128.783 1.00 72.45	С
ATOM		LYS A 529	13.658 32.014 128.150 1.00 72.88	Ο
		B LYS A 529		С
		G LYS A 529		С
ATOM		D LYS A 529	15.124 34.855 125.362 1.00 76.29	С
ATOM		E LYS A 529		С
		Z LYS A 529	17.601 34.302 125.151 1.00 80.14	N
ATOM		CYS A 530	15.153 32.854 129.573 1.00 75.18	N
ATOM		A CYS A 530	15.829 31.576 129.772 1.00 78.32	С
ATOM		CYS A 530	14.945 30,584 130.490 1.00 80.30	С
ATOM		CYS A 530	14.902 29.381 130.196 1.00 81.47	0
		B CYS A 530		С
		G ACYS A 530	18,275 32,752 129,297 0,50 79,21	S
		G BCYS A 530	17.568 30.622 131.680 0.50 81.24	S
		LYS A 531	14.102 31.009 131.421 1.00 82.32	N
			13.144 30.200 132.155 1.00 83.76	С
ATOM	1750 C	LYS A 531	11.970 29.841 131.246 1.00 85.00	С
		LYS A 531	11.021 29.148 131.602 1.00 85.73	Ο
<b>ATOM</b>	1752 C	B LYS A 531	12.572 30.964 133.355 1.00 83.88	С
<b>ATOM</b>	1753 C	G LYS A 531	13.345 30.854 134.647 1.00 84.87	С
<b>ATOM</b>	1754 C	D LYS A 531	14.805 31.287 134.574 1.00 85.69	С
<b>ATOM</b>	1757 N	ASN A 532	11.943 30.327 130.025 1.00 86.68	N
<b>ATOM</b>	1758 C	A ASN A 532	10.897 30.076 129.057 1.00 88.62	С
<b>ATOM</b>	1759 C	<b>ASN A 532</b>	9.561 30.539 129.591 1.00 87.46	С
ATOM	1760 O	ASN A 532	8.631 29.761 129.724 1.00 88.90	Ο
ATOM	1761 C	B ASN A 532	10.865 28.584 128.719 1.00 91.95	С
<b>ATOM</b>	1762 C	G ASN A 532	12.111 28.192 127.933 1.00 95.44	С
ATOM	1763 O	D1 ASN A 532	12.541 28.919 127.018 1.00 97.13	О
ATOM	1764 N	D2 ASN A 532	12.669 27.040 128.317 1.00 96.70	N
ATOM	1765 N	VAL A 533	9.437 31.803 129.937 1.00 85.64	N
ATOM	1766 C	A VAL A 533	8.226 32.396 130.477 1.00 84.02	С
ATOM		VAL A 533	7.754 33.510 129.545 1.00 83.66	С
		VAL A 533	6.622 33.965 129.431 1.00 84.28	О
		B VAL A 533	8.579 33.025 131.836 1.00 83.74	C
		G1 VAL A 533	7.314 33.478 132.539 1.00 84.23	С
		G2 VAL A 533	9.365 32.100 132.744 1.00 83.35	С
		VAL A 534	8.709 34.036 128.803 1.00 82.83	N
		A VAL A 534	8.538 35.100 127.846 1.00 82.58	С
		VAL A 534	8.243 34.525 126.465 1.00 82.12	C
		VAL A 534	8.956 33.657 125.956 1.00 81.14	0
		B VAL A 534	9.852 35.922 127.723 1.00 83.39	C
		G1 VAL A 534	9.874 36.971 126.614 1.00 83.09	C
		G2 VAL A 534	10.138 36.622 129.047 1.00 84.00	C
		PRO A 535	7.211 35.078 125.856 1.00 81.83	N
ATOM	1780 C	A PRO A 535	6.814 34.762 124.508 1.00 82.27	С

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ATOM	1781 C PRO A 535		С
<b>ATOM</b>	1782 O PRO A 535	8.852 35.993 123.727 1.00 81.80	Ο
		5.489 35.480 124.209 1.00 81.89	
ATOM	1784 CG PRO A 535	5.161 36.150 125.500 1.00 81.49	С
		6.365 36.127 126.413 1.00 81.75	
		7.710 34.667 122.314 1.00 84.28	N
		8.585 34.888 121.181 1.00 84.76	С
ATOM	1788 C LEU A 536	8.321 36.144 120.362 1.00 83.94	C
ATOM	1789 O LEU A 536	8.224 36.055 119.125 1.00 84.95	$\mathbf{O}_{\downarrow}$
		8.213 37.297 121.028 1.00 81.31	
		7.998 38.516 120.254 1.00 78.44	C
		9.356 38.798 119.616 1.00 76.32	
	1797 O TYR A 537		
ATOM	1798 CB TYR A 537	7.515 39.639 121.120 1.00 79.11	
		6.202 39.346 121.803 1.00 79.98	C
		5.051 39.111 121.078 1.00 80.95	
		6.097 39.316 123.180 1.00 80.52	C
		3.834 38.849 121.682 1.00 81.26	
ATOM	1803 CE2 TYR A 537	4.888 39.059 123.788 1.00 80.94	
ATOM	1804 CZ TYR A 537	3.759 38.826 123.052 1.00 81.36	C
		2.544 38.569 123.656 1.00 81.97	0
		9.336 38.912 118.299 1.00 74.66	N
		10.514 39.140 117.499 1.00 71.95	C
	1808 C ASP A 538		C
		12.485 40.348 117.818 1.00 66.05	0
ATOM	1810 CB ASP A 538	10.065 39.019 116.029 1.00 77.04	C
		10.164 37.552 115.613 1.00 81.25	С
		11.125 36.875 116.066 1.00 83.37	
		9.308 37.060 114.837 1.00 83.49	
		10.635 41.587 117.635 1.00 61.63	
		11.356 42.857 117.766 1.00 56.44	
	1816 C LEU A 539		C
	1817 O LEU A 539	13.082 43.499 119.280 1.00 56.68	0
	1818 CB LEU A 539	10.416 44.005 117.465 1.00 54.10	C
	1819 CG LEU A 539	10.884 45.430 117.325 1.00 51.84	C
	1820 CD1 LEU A 539	12.181 45.567 116.558 1.00 52.42	С
	1821 CD2 LEU A 539	9.833 46.284 116.643 1.00 50.66	C
	1822 N LEU A 540	11.279 42.532 120.186 1.00 55.25	N
	1823 CA LEU A 540	11.747 42.556 121.561 1.00 52.61	С
	1824 C LEUA 540	12.920 41.597 121.684 1.00 52.69 13.927 41.999 122.263 1.00 53.12	C
	1825 O LEU A 540	10.646 42.178 122.551 1.00 51.55	O C
	1826 CB LEU A 540	10.646 42.178 122.331 1.00 31.33	C
	1827 CG LEU A 540	10.979 42.209 124.044 1.00 30.31	C
	1828 CD1 LEU A 540 1829 CD2 LEU A 540	10.015 41.374 124.860 1.00 49.08	C
AIOM	1027 CD2 LEU A 340	10.013 41.374 124.600 1.00 49.08	C

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ΔΤΟΜ	1920 C SER B 305	27.429 71.556 157.295 1.00 88.55	С
		27.225 72.515 156.538 1.00 88.16	Ō
		25.569 69.949 156.772 1.00 88.41	C
ATOM	1923 OG SER B 305	26.477 69.152 156.035 1.00 87.79	0
	1924 N LEUB 306		N
	1925 CA LEU B 306	29,821 71.887 157.029 1.00 87.60	С
	1926 C LEUB 306		С
	1927 O LEUB 306		0
ATOM	1928 CB LEU B 306	31.152 71.166 157.258 1.00 88.10	С
	1932 N ALA B 307		N
		28.954 70.789 153.506 1.00 83.05	С
	1934 C ALA B 307		С
<b>ATOM</b>	1935 O ALA B 307	28.688 72.783 152.238 1.00 82.40	О
<b>ATOM</b>	1936 CB ALA B 307	28.050 69.587 153.251 1.00 83.80	C
	1937 N LEUB 308		N
	1938 CA LEUB 308	26.224 73.402 153.311 1.00 81.25	С
	1939 C LEUB 308		C
ATOM	1940 O LEUB 308	26.112 75.750 153.276 1.00 84.12	0
		24.833 73.206 153.918 1.00 80.91	C
		24.119 71.927 153.501 1.00 81.19	С
		22.625 72.029 153.804 1.00 82.22	С
		24.303 71.612 152.027 1.00 81.42	C
	1945 N SER B 309		N C
	1946 CA SER B 309 1947 C SER B 309	28.504 76.235 154.570 1.00 80.23 29.757 76.570 153.798 1.00 78.85	C
	1948 O SER B 309		0
ATOM		28.945 76.199 156.048 1.00 81.60	C
ATOM		27.839 75.621 156.755 1.00 84.43	
	1951 N LEUB 310		
ATOM	1957 CA LEUR 310	31.727 75.890 152.636 1.00 74.77	C
	1953 C LEUB 310		C
ATOM	1954 O LEUB 310	30.248 76.603 150.819 1.00 73.10	0
ATOM	1955 CB LEUB 310	32.577 74.676 152.338 1.00 74.13	C .
ATOM	1956 CG LEU B 310	32,501 73,548 153,358 1.00 73.86	С
ATOM	1957 CD1 LEU B 310	31.862 72.354 152.682 1.00 73.73	C
<b>ATOM</b>	1958 CD2 LEU B 310	33.893 73.207 153.878 1.00 74.39	С
<b>ATOM</b>	1959 N THR B 311	32.356 77.379 150.891 1.00 72.63	N
ATOM	1960 CA THR B 311	32,217 78,181 149,680 1,00 71,48	С
ATOM	1961 C THR B 311	32.717 77.311 148.556 1.00 70.23	С
	1962 O THR B 311	33.526 76.425 148.873 1.00 69.71	0
	1963 CB THR B 311	33.046 79.459 149.869 1.00 72.04	С
ATOM	1964 OG1 THR B 311	34.432 79.184 150.007 1.00 71.51	0
ATOM	1965 CG2 THR B 311	32.624 80.144 151.172 1.00 72.51	C
ATOM	1966 N ALA B 312	32.343 77.539 147.311 1.00 69.55	N
ATOM	1967 CA ALA B 312	32.847 76.686 146.239 1.00 69.89	C

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		154 371	
		34.355 76.490 146.399 1.00 70.66	С
ATOM		34.812 75.352 146.204 1.00 71.02	0
		32.533 77.194 144.852 1.00 69.74	C
	1971 N ASP B 313	35.109 77.532 146.738 1.00 71.01	N
		36.532 77.350 146.907 1.00 72.28	C
	1973 C ASP B 313		C O
		37.776 75.572 147.780 1.00 70.97 37.207 78.709 147.104 1.00 76.97	C
ATOM	1975 CD ASF B 313	37.316 79.339 145.715 1.00 81.71	Č
		37.885 78.667 144.807 1.00 83.39	Ö
		36.821 80.490 145.531 1.00 84.01	Ö
	1979 N GLN B 314	36.282 76.463 149.186 1.00 70.43	N
		36.617 75.551 150.272 1.00 70.03	С
	1981 C GLN B 314	36.258 74.111 149.897 1.00 68.40	С
ATOM	1982 O GLN B 314	37.035 73.183 150.134 1.00 68.40	0
ATOM	1983 CB GLN B 314	35.863 75.933 151.539 1.00 72.10	С
		35.710 77.430 151.674 1.00 74.15	С
		35.109 77.833 153.005 1.00 75.96	С
		33.942 78.211 153.112 1.00 77.07	0
		35.968 77.728 154.015 1.00 76.35	N
	1988 N MET B 315	35.068 73.967 149.304 1.00 65.55	N
	1989 CA MET B 315	34.585 72.674 148.838 1.00 62.07	C
	1990 C MET B 315	35.664 72.028 147.976 1.00 60.02	С
	1991 O MET B 315 1992 CB MET B 315	36.124 70.920 148.247 1.00 58.85 33.289 72.894 148.070 1.00 61.80	O C
	1992 CB MET B 315	32.588 71.654 147.554 1.00 62.43	C
		31.499 70.886 148.793 1.00 62.75	S
		32.375 69.332 148.932 1.00 62.81	Č
		36.101 72.735 146.936 1.00 58.75	N
		37.113 72.194 146.044 1.00 59.58	C
		38.356 71.690 146.767 1.00 60.61	С
<b>ATOM</b>	1999 O VAL B 316	38.881 70.619 146.456 1.00 61.28	0
<b>ATOM</b>	2000 CB VAL B 316	37.610 73.173 144.958 1.00 59.08	С
		38.727 72.541 144.132 1.00 58.28	С
		36.478 73.560 144.022 1.00 59.27	С
	2003 N SER B 317	38.877 72.498 147.672 1.00 61.25	N
	2004 CA SER B 317	40.097 72.148 148.395 1.00 61.71	C
	2005 C SER B 317	39.843 70.994 149.344 1.00 60.20	C
	2006 O SER B 317	40.676 70.092 149.474 1.00 60.58	0
	2007 CB SER B 317	40.539 73.355 149.236 1.00 64.18	C 0
	2008 OG SER B 317 2009 N ALA B 318	39.510 74.345 149.098 1.00 67.30 38.668 71.040 149.975 1.00 57.91	N
	2010 CA ALA B 318	38.335 69.952 150.891 1.00 56.48	C
	2011 C ALAB 318		c
	2011 C ALAB318 2012 O ALAB318	38.992 67.662 150.580 1.00 55.85	Ö
		11.11 1 100,000 1.00 00.00	_

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ATOM	2013	CB ALAB318	36.946 70.127 151.461 1.00 56.32	С
ATOM		N LEUB 319	37.855 68.687 148.891 1.00 54.38	N
ATOM		CA LEUB 319	37.824 67.501 148.044 1.00 53.50	C
ATOM		C LEU B 319	39.205 67.171 147.565 1.00 54.80	c
ATOM		O LEU B 319	39.674 66.048 147.650 1.00 54.87	Ö
ATOM		CB LEU B 319		C
		CG LEUB 319		Č
ATOM		CD1 LEU B 319	34.606 68.162 146.040 1.00 50.92	C
ATOM		CD2 LEU B 319	34.931 66.463 147.916 1.00 49.29	С
ATOM		N LEUB 320	39.921 68.193 147.116 1.00 57.27	N
ATOM		CA LEU B 320	41.298 68.008 146.647 1.00 58.44	С
ATOM		C LEUB 320	42.131 67.387 147.747 1.00 60.71	C
		O LEUB 320	43.023 66.589 147.492 1.00 61.28	Ö
ATOM		CB LEUB 320	41.847 69.356 146.194 1.00 57.26	C
ATOM		CG LEU B 320	41.571 69.548 144.707 1.00 57.56	Ċ
		CD1 LEU B 320	42.037 70.904 144.200 1.00 58.40	C
		CD2 LEU B 320	42.260 68.415 143.954 1.00 57.16	Ċ
ATOM		N ASP B 321	41.848 67.748 148.988 1.00 63.60	N
ATOM		CA ASP B 321	42.558 67.207 150.114 1.00 67.77	С
ATOM		C ASP B 321	42.264 65.767 150.479 1.00 66.98	С
		O ASP B 321	43.153 65.028 150.905 1.00 68.46	0
		CB ASP B 321	42.159 68.035 151.346 1.00 73.48	С
		CG ASP B 321	43.357 68.907 151.702 1.00 78.86	С
<b>ATOM</b>	2036	OD1 ASP B 321	44.358 68.838 150.933 1.00 80.91	0
<b>ATOM</b>	2037	OD2 ASP B 321	43.234 69.622 152.738 1.00 81.75	0
ATOM	2038	N ALA B 322	41.013 65.337 150.345 1.00 64.01	N
ATOM	2039	CA ALA B 322	40.651 63.979 150.713 1.00 60.43	С
ATOM	2040	C ALA B 322	41.260 62.949 149.783 1.00 59.13	С
ATOM	2041	O ALA B 322	41.306 61.772 150.141 1.00 58.64	Ο
ATOM	2042	CB ALA B 322	39.130 63.958 150.695 1.00 59.91	С
ATOM	2043	N GLUB 323	41.711 63.341 148.596 1.00 57.38	N
ATOM	2044	CA GLU B 323	42.265 62.393 147.650 1.00 56.07	С
ATOM	2045	C GLU B 323	43.165 61.402 148.323 1.00 55.73	С
ATOM	2046	O GLU B 323	43.982 61.745 149.167 1.00 58.17	0
		CB GLU B 323	42.959 63.161 146.539 1.00 56.37	C
ATOM	2048	CG GLU B 323	41.903 63.704 145.555 1.00 57.34	С
		CD GLU B 323	41.427 62.553 144.690 1.00 58.29	C
		OE1 GLU B 323	42.238 61.857 144.034 1.00 59.37	0
		OE2 GLU B 323	40.222 62.286 144.663 1.00 58.17	0
		N PRO B 324	43.009 60.136 148.013 1.00 55.05	N
		CA PRO B 324	43.797 59.044 148.563 1.00 54.36	С
		C PRO B 324	45.142 58.976 147.861 1.00 55.37	C
		O PRO B 324	45.401 59.613 146.835 1.00 56.48	0
		CB PRO B 324	43.006 57.765 148.252 1.00 53.47	C
ATOM	2057	CG PRO B 324	42.269 58.183 147.016 1.00 53.95	С

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ATOM	2058 CD PRO B 324	42.056 59.670 146.998 1.00 54.63	С
		46.032 58.173 148.383 1.00 55.73	N
<b>ATOM</b>	2060 CA PRO B 325	47.354 57.952 147.848 1.00 56.79	С
ATOM	2061 C PRO B 325	47.354 57.952 147.848 1.00 56.79 47.235 57.105 146.593 1.00 58.51	С
ATOM	2062 O PROB 325	46.186 56.455 146.548 1.00 59.42	0
		48.084 57.111 148.908 1.00 56.61	C
		46.945 56.405 149.583 1.00 56.03	С
		45.784 57.370 149.587 1.00 56.49	С
		48.185 57.070 145.677 1.00 59.89	N
		48.081 56.220 144.497 1.00 61.78	
		48.771 54.904 144.848 1.00 60.68	
ATOM	2069 O ILEB 326	49.919 55.033 145.279 1.00 62.66	0
ATOM	2070 CB ILE B 320	48.7/4 30.083 143.208 1.00 65.00	C
ATOM	2071 CG1 ILE B 326	48.774 56.685 143.208 1.00 65.00 50.257 57.062 143.384 1.00 68.09 48.016 57.832 142.521 1.00 64.84	C C
ATOM	2072 CO2 ILE B 326	50.668 57.986 144.527 1.00 69.81	C
		48.160 53.747 144.735 1.00 59.06	
		48.909 52.546 145.122 1.00 58.44	
		49.829 52.088 144.008 1.00 58.98	c
ATOM	2077 O LEUB 327	49.826 52.665 142.938 1.00 59.09	Ö
		47.876 51.501 145.502 1.00 57.19	
ATOM	2079 CG LEU B 327	46,808 51,909 146,493 1,00 56,05	С
ATOM	2080 CD1 LEU B 327	46.233 50.637 147.122 1.00 55.97 47.321 52.844 147.568 1.00 55.58	С
ATOM	2081 CD2 LEU B 327	47.321 52.844 147.568 1.00 55.58	С
ATOM	2082 N TYR B 328	50.628 51.067 144.227 1.00 60.54	N
		51.514 50.508 143.229 1.00 62.26	
		51.076 49.047 143.140 1.00 63.10	С
ATOM	2085 O TYR B 328	50.702 48.523 144.172 1.00 62.38	0
ATOM	2086 CB TYR B 328	52.998 50.527 143.560 1.00 63.28 53.619 51.884 143.281 1.00 64.36	C
ATOM	2087 CG TYKB 328	53.619 51.884 143.281 1.00 64.36	C
	2089 CD2 TYR B 328	53.626 52.866 144.259 1.00 64.71	C
	2090 CE1 TYR B 328	54.168 52.171 142.050 1.00 64.48 54.182 54.104 144.018 1.00 65.70	C C
	2091 CE2 TYR B 328	54.716 53.413 141.810 1.00 65.61	C
	2092 CZ TYR B 328	54.728 54.375 142.788 1.00 66.10	c
	2093 OH TYR B 328	55.288 55.604 142.502 1.00 67.55	Ö
	2094 N SER B 329	51.102 48.465 141.959 1.00 65.42	N
	2095 CA SER B 329	50.677 47.083 141.860 1.00 67.55	C
ATOM	2096 C SER B 329	51.719 46.193 142.513 1.00 70.65	С
ATOM	2097 O SER B 329	52.883 46.548 142.456 1.00 71.72	0
	2098 CB SER B 329	50.548 46.669 140.404 1.00 66.96	С
	2099 OG SER B 329	50.526 45.240 140.433 1.00 67.55	0
	2100 N GLUB 330	51.326 45.087 143.091 1.00 75.08	N
	2101 CA GLUB 330	52.235 44.145 143.719 1.00 79.78	C
ATOM	2102 C GLU B 330	53.117 43.539 142.618 1.00 81.27	С

43.342 35.081 132.949 1.00 74.09 ATOM 2127 CA GLU B 339 C 43.526 35.122 134.469 1.00 72.45 C ATOM 2128 C GLUB 339 0 ATOM 2129 O GLUB 339 43.440 36.205 135.065 1.00 72.49 C 42.301 34.079 132.505 1.00 74.26 ATOM 2130 CB GLU B 339 ATOM 2131 CG GLU B 339 41.030 33.874 133.294 1.00 74.49 C 39.898 33.645 132.292 1.00 75.67 C ATOM 2132 CD GLU B 339 ATOM 2133 OE1 GLU B 339 39,740 34,445 131,339 1.00 75.56 0 39.164 32.644 132.444 1.00 76.73 0 ATOM 2134 OE2 GLU B 339 43.858 33.991 135.105 1.00 70.10 ATOM 2135 N ALA B 340 N ATOM 2136 CA ALAB 340 44.067 33.983 136.538 1.00 68.16 C ATOM 2137 C ALA B 340 45.121 34.958 137.043 1.00 67.65 0 ATOM 2138 O ALA B 340 44.825 35.704 137.990 1.00 67.91 C ATOM 2139 CB ALA B 340 44.424 32.585 136.991 1.00 67.98 ATOM 2140 N SER B 341 46.321 34.993 136.474 1.00 66.66 N 47.329 35.924 136.982 1.00 65.93 C ATOM 2141 CA SER B 341 C ATOM 2142 C SER B 341 46.854 37.355 136.798 1.00 65.12 ATOM 2143 O SER B 341 47.080 38.127 137.749 1.00 65.86 0 C ATOM 2144 CB SER B 341 48.696 35.668 136.372 1.00 67.56 ATOM 2145 OG SER B 341 49.175 36.672 135.498 1.00 70.60 0 46.221 37.699 135.663 1.00 63.28 N ATOM 2146 N MET B 342 ATOM 2147 CA MET B 342 45.773 39.078 135.485 1.00 61.89 C

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ATOM	2148 C MET B 342	44.654 39.478 136.444 1.00 60.47	С
ATOM	2149 O MET B 342	44.752 40.481 137.159 1.00 60.54	0
ATOM	2150 CB MET B 342	45.270 39.454 134.093 1.00 61.38	С
ATOM	2151 CG MET B 342	45.270 39.454 134.093 1.00 61.38 45.272 40.980 134.038 1.00 62.54 45.488 41.560 132.349 1.00 66.23	С
ATOM	2152 SD MET B 342	45.488 41.560 132.349 1.00 66.23	S
	2153 CE MET B 342		
	2154 N MET B 343	43.602 38.664 136.486 1.00 58.53	N
	2155 CA MET B 343	42.495 38.932 137.396 1.00 57.10	С
	2156 C MET B 343		C
	2157 O MET B 343		0
		41.513 37.780 137.393 1.00 56.26	C
ATOM	2159 CG MET B 343	40.589 37.839 136.195 1.00 56.11	C
		39.684 39.386 136.078 1.00 56.84	S
	2161 CE MET B 343		C
	2162 N GLY B 344 2163 CA GLY B 344		N
	2164 C GLY B 344	44.679 38.468 140.491 1.00 54.71	C
	2165 O GLY B 344	45.227 39.869 140.678 1.00 53.89 44.813 40.511 141.639 1.00 53.84	C O
ATOM			N
		46.621 41.760 140.042 1.00 54.09	C
		45.532 42.824 140.167 1.00 53.00	c
		45.490 43.579 141.140 1.00 53.38	Ö
		47.408 42.284 138.844 1.00 55.45	Č
ATOM	2171 CG LEUB 345	48.757 41.626 138.559 1.00 57.40	Č
		48.684 41.033 137.157 1.00 57.22	C
<b>ATOM</b>	2173 CD2 LEU B 345	49.874 42.651 138.738 1.00 57.21	С
ATOM	2174 N LEUB 346	44.701 42.843 139.117 1.00 50.42	N
ATOM	2175 CA LEU B 346	43.595 43.791 139.045 1.00 48.04	С
	2176 C LEUB 346		С
	2177 O LEUB 346	42.509 44.746 141.008 1.00 46.14	0
ATOM		42.828 43.449 137.782 1.00 47.72	C
	2179 CG LEUB 346	43.598 43.886 136.509 1.00 48.42	C
	2180 CD1 LEUB 346	42.660 43.796 135.311 1.00 48.05	C
	2181 CD2 LEU B 346	44.224 45.266 136.613 1.00 47.09	C
	2182 N THR B 347	42.349 42.553 140.628 1.00 46.25	N
	2183 CA THR B 347	41.549 42.288 141.820 1.00 46.10	C
	2184 C THR B 347 2185 O THR B 347	42.238 42.666 143.100 1.00 47.12	C
	2186 CB THR B 347	41.675 43.312 144.002 1.00 47.76	O C
	2187 OG1 THR B 347	41.162 40.813 141.668 1.00 45.79 39.731 40.798 141.443 1.00 47.18	
	2188 CG2 THR B 347	41.638 39.936 142.757 1.00 44.47	O C
ATOM		43.516 42.349 143.245 1.00 48.37	N
	2190 CA ASN B 348	44.312 42.696 144.422 1.00 47.96	C
	2191 C ASN B 348	44.383 44.213 144.550 1.00 46.69	c
	2192 O ASN B 348	44.120 44.863 145.568 1.00 46.53	Ö
		11.120 11.003 113.300 1.00 TO.33	•

			159/3+1	
ATOM	2193	CB ASN B 348	45.687 42.077 144.255 1.00 50.12	С
ATOM	2194	CG ASN B 348	46.646 42.472 145.355 1.00 53.52	С
<b>ATOM</b>	2195	OD1 ASN B 348	47.392 43.475 145.293 1.00 55.04	О
ATOM	2196	ND2 ASN B 348	46.576 41.621 146.382 1.00 54.64	Ν
ATOM	2197	N LEU B 349	44.729 44.861 143.440 1.00 45.19	N
ATOM	2198	CA LEU B 349	44.827 46.327 143.461 1.00 44.31	С
ATOM	2199	C LEU B 349	43.516 46.920 143.946 1.00 42.73	С
ATOM	2200	O LEU B 349	43,496 47,803 144,782 1,00 41.58	0
<b>ATOM</b>	2201	CB LEU B 349	45.260 46.806 142.070 1.00 44.84	С
<b>ATOM</b>	2202	CG LEUB 349	45.463 48.314 141.897 1.00 45.41	С
<b>ATOM</b>	2203	CD1 LEU B 349	46.548 48.802 142.850 1.00 45.52	С
ATOM	2204	CD2 LEU B 349	45.780 48.735 140.467 1.00 44.75	С
<b>ATOM</b>	2205	N ALA B 350	42.387 46.437 143.433 1.00 42.61	N
ATOM	2206	CA ALA B 350	41.064 46.936 143.776 1.00 42.37	С
ATOM	2207	C ALA B 350	40.836 46.794 145.268 1.00 42.95	С
ATOM	2208	O ALA B 350	40.543 47.737 146.002 1.00 41.96	Ο
ATOM	2209	CB ALA B 350	39.967 46.201 143.010 1.00 41.65	С
ATOM	2210	N ASP B 351	41.030 45.560 145.745 1.00 44.56	N
ATOM	2211	CA ASP B 351	40.862 45.330 147.181 1.00 46.40	С
ATOM	2212	C ASP B 351	41.664 46.319 148.016 1.00 46.43	С
ATOM	2213	O ASP B 351	41.230 46.750 149.090 1.00 47.39	Ο
ATOM	2214	CB ASP B 351	41.238 43.886 147.491 1.00 48.98	С
ATOM	2215	CG ASP B 351	41.021 43.624 148.973 1.00 51.85	С
ATOM	2216	OD1 ASP B 351	39.868 43.494 149.431 1.00 52.63	0
ATOM	2217	OD2 ASP B 351	42.069 43.568 149.663 1.00 54.48	0
ATOM	2218	N ARG B 352	42.857 46.724 147.596 1.00 46.00	N
ATOM	2219	CA ARG B 352	43.654 47.672 148.350 1.00 45.92	С
ATOM	2220		43.139 49.091 148.289 1.00 45.41	С
ATOM	2221	O ARG B 352	43.092 49.793 149.312 1.00 46.29	0
ATOM	2222		45.081 47.581 147.832 1.00 46.64	C
ATOM	2223	CG ARG B 352	45.757 46.326 148.369 1.00 48.12	C
ATOM		CD ARG B 352		С
ATOM		NE ARG B 352	47.831 46.493 147.298 1.00 52.10	N
		CZ ARG B 352	48.655 47.337 146.661 1.00 52.15	C
		NHI ARG B 352	49.011 48.472 147.259 1.00 50.48	N
		NH2 ARG B 352	49.015 46.878 145.451 1.00 51.51	N
ATOM		N GLU B 353	42.701 49.536 147.119 1.00 44.33	N
ATOM		CA GLU B 353	42.161 50.889 146.991 1.00 43.49	C
		C GLUB 353	40.862 51.033 147.789 1.00 43.42	C
ATOM		O GLU B 353	40.503 52.128 148.220 1.00 42.92	0
		CB GLUB 353	41.848 51.196 145.537 1.00 42.87	C
ATOM		CG GLU B 353	42.933 50.836 144.558 1.00 43.52	C
ATOM		CD GLU B 353	42.710 51.456 143.201 1.00 44.16	C
		OE1 GLU B 353	42.597 52.674 143.043 1.00 43.57	0
ATOM	2237	OE2 GLU B 353	42.628 50.706 142.214 1.00 45.84	0

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			160/371	
ATOM	2238	N LEU B 354	40.153 49.915 147.992 1.00 42.83	N
ATOM	2239	CA LEUB 354	38.900 49.915 148.712 1.00 42.73	С
ATOM	2240	C LEU B 354	39.083 50.455 150.110 1.00 43.31	С
ATOM	2241	O LEU B 354	38.270 51.257 150.594 1.00 43.47	0
ATOM	2242	CB LEUB 354	38.210 48.546 148.710 1.00 41.85	С
ATOM	2243	CG LEUB 354	37.399 48.461 147.392 1.00 41.01	С
ATOM	2244	CD1 LEU B 354	37.232 47.020 147.007 1.00 42.17	С
ATOM	2245	CD2 LEU B 354	36.098 49.201 147.579 1.00 40.64	С
ATOM	2246	N VAL B 355	40.192 50.012 150.697 1.00 43.66	N
ATOM	2247	CA VALB 355	40.513 50.540 152.037 1.00 43.57	С
ATOM	2248	C VAL B 355	40.640 52.049 151.989 1.00 43.49	С
ATOM	2249	O VAL B 355	39.931 52.791 152.667 1.00 44.38	Ο
ATOM	2250	CB VAL B 355	41.822 49.887 152.485 1.00 42.19	С
ATOM	2251	CG1 VAL B 355	42.185 50.377 153.841 1.00 41.86	С
ATOM	2252	CG2 VAL B 355	41.536 48.388 152.492 1.00 43.55	С
ATOM	2253	N HIS B 356	41.502 52.573 151.138 1.00 43.64	N
ATOM	2254	CA HIS B 356	41.663 54.020 151.046 1.00 44.98	С
ATOM	2255	C HIS B 356	40.354 54.684 150.718 1.00 44.85	С
ATOM	2256	O HIS B 356	40.075 55.789 151.171 1.00 44.94	0
ATOM	2257	CB HIS B 356	42.746 54.342 150.000 1.00 48.00	С
ATOM		CG HIS B 356	44.039 53.806 150.549 1.00 50.79	С
ATOM		ND1 HIS B 356	44.987 54.578 151.156 1.00 51.64	N
ATOM		CD2 HIS B 356	44.492 52.531 150.622 1.00 52.67	С
ATOM	2261	CE1 HIS B 356	45.975 53.804 151.555 1.00 52.82	С
ATOM		NE2 HIS B 356	45.717 52.545 151.255 1.00 53.04	N
		N MET B 357	39.527 54.042 149.887 1.00 45.52	N
ATOM		CA MET B 357	38.258 54.585 149.440 1.00 43.50	С
ATOM		C MET B 357	37.366 54.938 150.612 1.00 43.20	C
ATOM			36.851 56.042 150.626 1.00 44.03	0
		CB MET B 357	37.424 53.666 148.547 1.00 42.56	C
		CG MET B 357	36.286 54.506 147.943 1.00 42.38	C
ATOM			35.245 53.437 146.919 1.00 43.60	S
ATOM		CE MET B 357	36.318 53.100 145.547 1.00 42.88	C
		N ILEB 358	37.213 53.978 151.513 1.00 42.20	N
		CA ILE B 358	36.378 54.184 152.687 1.00 40.88	C
		C ILEB 358	36.869 55.416 153.422 1.00 42.97	C
		O ILEB 358	36.054 56.284 153.754 1.00 43.92	0
		CB ILE B 358	36.483 52.950 153.581 1.00 39.18	С
		CG1 ILE B 358	35.909 51.759 152.836 1.00 39.34	C
		CG2 ILE B 358	35.767 53.190 154.879 1.00 39.09	C C
		CD1 ILE B 358	36.019 50.424 153.527 1.00 39.80	N
		N ASN B 359	38.174 55.520 153.673 1.00 44.15	C
ATOM		CA ASN B 359	38.709 56.695 154.338 1.00 45.85	
ATOM	2281		38.317 57.963 153.628 1.00 44.78	C
ATOM	2282	O ASN B 359	37.738 58.868 154.190 1.00 45.76	0

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***	70,500		161/371	
ATOM	2283	CB ASN B 359	40.230 56.589 154.376 1.00 50.87	С
		CG ASN B 359	40.498 55.579 155.477 1.00 56.26	С
		OD1 ASN B 359	40.076 55.925 156.602 1.00 61.30	Ο
		ND2 ASN B 359	41.104 54.423 155.259 1.00 57.59	N
		N TRP B 360	38.598 58.043 152.346 1.00 44.00	N
ATOM	2288	CA TRP B 360	38.268 59.171 151.512 1.00 42.58	С
<b>ATOM</b>	2289	C TRP B 360	36.806 59.546 151.631 1.00 42.49	С
<b>ATOM</b>		O TRP B 360	36.410 60.691 151.727 1.00 42.71	0
		CB TRP B 360	38.544 58.717 150.069 1.00 42.21	C
		CG TRP B 360		C
		CD1 TRP B 360	38.328 60.905 148.764 1.00 42.29	C
		CD2 TRP B 360	36.667 59.443 148.365 1.00 42.41	C
		NEI TRP B 360	37.449 61.447 147.877 1.00 43.09	N
		CE2 TRP B 360	36.430 60.586 147.599 1.00 42.27	C C
		CE3 TRP B 360	35.760 58.378 148.288 1.00 42.53	C
		CZ2 TRP B 360	35.342 60.733 146.752 1.00 42.40	C
		CZ3 TRP B 360	34.674 58.519 147.451 1.00 43.36 34.462 59.688 146.688 1.00 43.36	C
		CH2 TRP B 360	35.898 58.584 151.574 1.00 44.00	N
		N ALA B 361		C
		CA ALA B 361 C ALA B 361	34.177 59.629 152.930 1.00 46.34	c
		O ALA B 361	33.398 60.572 152.903 1.00 45.79	Ö
		CB ALA B 361	33.690 57.534 151.609 1.00 44.61	Č
		N LYS B 362	34.804 59.320 154.051 1.00 48.42	N
		CA LYS B 362	34.581 60.009 155.298 1.00 51.41	С
		C LYS B 362	34.844 61.494 155.237 1.00 51.60	С
		O LYS B 362	34.262 62.243 156.028 1.00 52.45	0
		CB LYS B 362	35.368 59.329 156.429 1.00 53.83	, <b>C</b>
		CG LYS B 362	34.783 57.948 156.761 1.00 56.54	С
<b>ATOM</b>	2312	CD LYS B 362	33.429 58.076 157.442 1.00 58.88	С
<b>ATOM</b>	2313	CE LYS B 362		С
ATOM	2314	NZ LYS B 362	32.112 57.527 159.530 1.00 61.36	N
		N ARG B 363	35.659 61.990 154.354 1.00 51.98	N
		CA ARG B 363	35.974 63.383 154.183 1.00 53.74	С
		C ARG B 363	35.176 64.086 153.096 1.00 52.36	C
ATOM			35.421 65.265 152.810 1.00 53.34	0
		CB ARG B 363	37.445 63.546 153.759 1.00 57.28	C
		CG ARG B 363	38.196 62.254 153.990 1.00 63.66	C C
		CD ARG B 363	38.649 62.308 155.471 1.00 69.44	N
		NE ARG B 363	39.675 63.365 155.438 1.00 74.98	C
		CZ ARG B 363	40.834 63.136 154.780 1.00 78.56 41.049 61.949 154.177 1.00 79.07	N
		NH1 ARG B 363	41.730 64.142 154.772 1.00 80.01	N
		NH2 ARG B 363	34.268 63.458 152.393 1.00 50.64	N
		N VAL B 364 CA VAL B 364	33.536 64.203 151.351 1.00 48.57	Ċ
ATOM	-24/	CA VAL D 304	JJ.JJU UT.20J IJI.JJI 1.00 T0.J/	J

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ATOM	2328	C VAL B 364	32.516 64.992 152.132 1.00 48.30	С
ATOM		O VAL B 364	31.679 64.424 152.834 1.00 49.68	Ο
ATOM	2330	CB VAL B 364	32.933 63.200 150.360 1.00 47.31	С
ATOM	2331	CG1 VAL B 364	31.906 63.840 149.457 1.00 46.60	С
ATOM	2332	CG2 VAL B 364	34.069 62.557 149.571 1.00 46.35	С
ATOM	2333	N PRO B 365	32.542 66.287 152.091 1.00 47.88	N
ATOM		CA PRO B 365	31.625 67.148 152.817 1.00 47.75	С
ATOM	2335	C PRO B 365	30.208 66.645 152.701 1.00 47.86	С
ATOM	2336	O PRO B 365	29.722 66.392 151.609 1.00 48.96	0
ATOM	2337	CB PRO B 365	31.788 68.552 152.204 1.00 47.58	С
ATOM	2338	CG PRO B 365	33.260 68.466 151.902 1.00 49.17	С
ATOM	2339	CD PRO B 365	33.509 67.057 151.312 1.00 48.98	С
<b>ATOM</b>	2340	N GLY B 366	29.537 66.463 153.821 1.00 48.34	N
<b>ATOM</b>	2341	CA GLY B 366	28.168 66.023 153.933 1.00 48.09	С
<b>ATOM</b>	2342	C GLY B 366	27.949 64.535 154.121 1.00 47.88	С
<b>ATOM</b>	2343	O GLY B 366	26.864 64.089 154.545 1.00 48.29	0
ATOM	2344	N PHE B 367	28.970 63.754 153.775 1.00 46.58	N
ATOM	2345	CA PHE B 367	28.849 62.306 153.856 1.00 46.69	С
<b>ATOM</b>	2346	C PHE B 367	28.516 61.780 155.244 1.00 46.32	С
ATOM	2347	O PHE B 367	27.608 61.036 155.593 1.00 44.65	0
ATOM	2348	CB PHE B 367	30.145 61.654 153.357 1.00 45.74	С
<b>ATOM</b>	2349	CG PHE B 367	30.040 60.160 153.204 1.00 45.19	С
ATOM	2350	CD1 PHE B 367	29.373 59.598 152.150 1.00 44.90	С
ATOM	2351	CD2 PHE B 367	30.613 59.325 154.144 1.00 45.86	С
ATOM	2352	CE1 PHE B 367	29.287 58.234 152.008 1.00 46.05	С
ATOM	2353	CE2 PHE B 367	30.537 57.958 154.029 1.00 46.38	С
ATOM		CZ PHE B 367	29.875 57.405 152.947 1.00 46.68	С
ATOM		N VAL B 368	29.358 62.254 156.134 1.00 47.15	N
ATOM		CA VAL B 368	29.376 61.923 157.550 1.00 48.33	С
ATOM		C VALB 368	28.103 62.324 158.245 1.00 49.61	C
ATOM		O VAL B 368	27.813 61.753 159.307 1.00 51.30	0
ATOM		CB VAL B 368	30.647 62.529 158.162 1.00 47.39	C
ATOM		CG1 VAL B 368	30.341 63.282 159.413 1.00 47.29	C
		CG2 VAL B 368	31.671 61.416 158.296 1.00 46.89	C
ATOM		N ASP B 369	27.323 63.233 157.685 1.00 50.09	N
		CA ASP B 369	26.035 63.587 158.254 1.00 50.46	С
		C ASP B 369	25.034 62.476 157.971 1.00 48.55	C
		O ASP B 369	23.922 62.589 158.461 1.00 50.33	0
ATOM		CB ASP B 369	25.475 64.892 157.668 1.00 53.89	C
ATOM		CG ASP B 369	26.430 66.074 157.769 1.00 58.03	C
		OD1 ASP B 369	27.112 66.330 158.802 1.00 59.26	0
ATOM		OD2 ASP B 369	26.554 66.855 156.780 1.00 59.49	0
ATOM		N LEUB 370	25.222 61.420 157.221 1.00 47.05	N
ATOM		CA LEUB 370	24.202 60.401 156.985 1.00 45.34	C
ATOM	2372	C LEU B 370	24.280 59.335 158.062 1.00 43.86	С

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ATOM	2373	O LEUB 370	25,306 59,324 158.740 1.00 44.04	0
ATOM		CB LEU B 370		С
ATOM		CG LEU B 370	24.312 60.763 154.454 1.00 46.82	С
ATOM		CDI LEU B 370	24.605 60.125 153.107 1.00 46.43	С
ATOM		CD2 LEU B 370	22.869 61.283 154.518 1.00 46.50	С
ATOM		N THR B 371	23.292 58.494 158.263 1.00 41.90	N
ATOM		CA THR B 371	23.420 57.495 159.308 1.00 42.13	С
ATOM		C THR B 371	24,521 56.534 158.912 1.00 43.67	С
ATOM		O THR B 371	24.823 56.337 157.727 1.00 44.74	0
ATOM		CB THR B 371	22.120 56.701 159.395 1.00 42.81	С
ATOM		OG1 THR B 371	21.749 56.371 158.054 1.00 44.14	O
ATOM		CG2 THR B 371	20.990 57.552 159.918 1.00 43.46	С
ATOM		N LEUB 372	25.132 55.886 159.899 1.00 44.52	N
ATOM		CA LEU B 372	26,204 54,944 159,612 1,00 44,27	C
ATOM		C LEU B 372	25.785 53.935 158.562 1.00 45.75	С
		O LEUB 372	26.637 53.676 157.691 1.00 46.87	Ο
		CB LEU B 372	26.618 54.282 160.915 1.00 43.07	С
ATOM	2390	CG LEU B 372	27.311 55.225 161.889 1.00 42.80	С
<b>ATOM</b>	2391	CD1 LEU B 372	27.664 54.482 163.168 1.00 43.31	С
ATOM	2392	CD2 LEU B 372	28.594 55.751 161.277 1.00 43.66	С
<b>ATOM</b>	2393	N HIS B 373	24.566 53.395 158.585 1.00 45.98	N
ATOM	2394	CA HISB 373	24.203 52.417 157.564 1.00 47.04	С
<b>ATOM</b>	2395	C HIS B 373	24.055 53.084 156.212 1.00 46.53	С
ATOM		O HIS B 373	24.487 52.447 155.220 1.00 47.00	O
ATOM	2397	CB HIS B 373	23.005 51.585 157.954 1.00 49.76	C
ATOM	2398	CG HISB 373	23.350 50.587 159.002 1.00 53.39	C
ATOM		ND1 HIS B 373	23.065 50.720 160.354 1.00 55.19	N
		CD2 HIS B 373	23.978 49.400 158.890 1.00 54.94	C
		CE1 HIS B 373	23.503 49.646 161.009 1.00 55.80	C
		NE2 HIS B 373	24.083 48.817 160.140 1.00 56.63	N
		N ASP B 374	23,537 54,308 156,149 1.00 44,27	N
		CA ASP B 374	23.478 54.919 154.815 1.00 44.35	C
		C ASP B 374	24.846 55.118 154.197 1.00 43.97	C
		O ASP B 374	24.956 54.968 152.974 1.00 43.72	O C
		CB ASP B 374		C
		CG ASP B 374	21,223 55,703 155,009 1,00 48,08 21,024 54,468 154,829 1,00 49,35	o
		OD1 ASP B 374	20.292 56.479 155.299 1.00 49.88	0
		OD2 ASP B 374	25.862 55.435 155.001 1.00 43.23	N
		N GLNB 375	27.195 55.584 154.434 1.00 43.62	C
		CA GLN B 375	27.193 33.384 134.434 1.00 43.02 27.589 54.230 153.874 1.00 44.32	c
		C GLN B 375 O GLN B 375	27.950 54.150 152.690 1.00 46.72	Ö
ATOM		CB GLN B 375	28.180 56.051 155.476 1.00 44.31	C
		CG GLN B 375	27.735 57.373 156.082 1.00 46.41	Č
			28.564 57.807 157.274 1.00 46.26	c
ATOM	41/	CD GLN B 375	20.304 37.607 137.274 1.00 40.20	C

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ΔΤΟΜ	2419 OE1 CINB 375	29.742 57.477 157.379 1.00 47.15	0
ATOM	2416 OEI GLN B 375	27.931 58.543 158.158 1.00 45.51	N
		27.483 53.136 154.625 1.00 42.98	
ATOM	2421 CA VAL B 376	27.843 51.849 154.027 1.00 42.65	C
ATOM	2422 C VAL B 376	27.054 51.662 152.740 1.00 43.08	С
ATOM	2423 O VAL B 376	27.611 51.284 151.714 1.00 43.58	0
		27.640 50.677 154.989 1.00 42.62	С
<b>ATOM</b>	2425 CG1 VAL B 376	28.412 49.481 154.467 1.00 42.57	С
		28.137 51.017 156.375 1.00 41.75	С
		25.753 51.934 152.711 1.00 44.02	N
		24.981 51.805 151.468 1.00 44.64	С
ATOM	2429 C HIS B 377	25.600 52.635 150.364 1.00 43.12	C
ATOM	2430 O HIS B 377	26.019 51.995 149.384 1.00 43.78	
ATOM	2431 CB HIS B 377	23.497 52.076 151.711 1.00 46.21	C
		22.607 52.039 150.512 0.50 44.35	C
		22.947 50.949 152.558 0.50 50.29	
ATOM	2434 ND1AHIS B 377	22.247 50.853 149.916 0.50 43.89	N
ATOM	2435 ND1BHIS B 377	22.350 51.163 153.793 0.50 51.12	N
ATOM	2430 CD2AHIS B 377	22.003 53.020 149.793 0.50 44.38 22.919 49.600 152.345 0.50 51.17	C C
ATOM	2437 CD2DIII3 D 377	21.466 51.118 148.877 0.50 43.90	C
		21.965 50.003 154.308 0.50 51.18	
		21.304 52.423 148.768 0.50 43.73	
ATOM	2441 NE2BHIS B 377	22.299 49.039 153.458 0.50 51.65	N
ATOM	2442 N LEUB 378	25.768 53.948 150.396 1.00 41.23	N
		26.408 54.598 149.239 1.00 40.29	С
		27.727 53.934 148.847 1.00 39.27	С
		28.095 53.717 147.675 1.00 37.62	0
<b>ATOM</b>	2446 CB LEUB 378	26.539 56.096 149.487 1.00 40.75	С
ATOM	2447 CG LEUB 378	25.290 56.820 149.987 1.00 40.78	С
ATOM	2448 CD1 LEU B 378	25.562 58.302 150.166 1.00 40.54	C
	2449 CD2 LEU B 378		С
	2450 N LEUB 379	28.540 53.551 149.829 1.00 38.80	N
	2451 CA LEUB 379	29.812 52.924 149.510 1.00 38.53	C
	2452 C LEUB 379	29.569 51.668 148.715 1.00 39.41	C
	2453 O LEUB 379	30.062 51.582 147.601 1.00 39.29	0
	2454 CB LEUB 379	30.626 52.631 150.754 1.00 37.75	C C
	2455 CG LEU B 379 2456 CD1 LEU B 379	31.544 53.840 151.017 1.00 38.48 32.100 53.599 152.411 1.00 40.54	C
	2457 CD2 LEU B 379	32.609 54.029 149.951 1.00 36.12	C
	2458 N GLUB 380	28.775 50.744 149.280 1.00 40.40	N
ATOM		28.481 49.507 148.576 1.00 40.60	C
ATOM		27.932 49.823 147.180 1.00 42.38	c
	2461 O GLUB 380	28.273 49.192 146.186 1.00 41.89	Ö
	2462 CB GLUB 380	27.496 48.721 149.377 1.00 39.04	C
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4 TO 1	2462 CG GIII B 380	28.010 48.175 150.668 1.00 43.02	С
ATOM	2464 CD GIII B 380	26.849 47.489 151.386 1.00 46.45	
ATOM	2465 OF1 GLUB 380	25.689 47.970 151.219 1.00 48.79	O
ATOM	2466 OE2 GLUB 380	27.057 46.480 152.108 1.00 47.08	Ö
	2467 N CYS B 381		N
ATOM	2407 N C13 B 361	26.504 51.108 145.760 1.00 46.42	Ċ
			c
	2469 C CYS B 381		Ö
ATOM	2470 U CISB 361	27.485 51.113 143.630 1.00 42.52 25.216 51.950 145.913 1.00 50.98	C
ATOM	24/1 CB CYS B 381	23.759 50.890 145.506 1.00 62.03	
ATOM	24/2 SG CIS B 361	28.335 52.615 145.072 1.00 42.25	N
ATOM	2475 N ALAB 382	28,333 32,613 143,072 1.00 42,23	C
		29.254 53.184 144.104 1.00 39.67 30.697 52.743 144.082 1.00 39.72	C
	2475 C ALA B 382		0
ATOM	2476 U ALAB 382	31.482 53.339 143.340 1.00 39.67	C
		29.325 54.671 144.482 1.00 38.16 31.121 51.713 144.797 1.00 39.88	N
	2478 N TRP B 383		C
ATOM	2479 CA TRP B 383	32.543 51.357 144.827 1.00 39.09	C
ATOM	2480 C TRP B 383	33.224 51.210 143.495 1.00 39.22	o
ATOM	2481 U TRP B 383	34.192 51.900 143.161 1.00 39.38	C
ATOM	2482 CB TRP B 383	32.724 50.169 145.722 1.00 38.40 32.290 48.861 145.180 1.00 37.57	C
ATOM	2483 CG TRP B 383	32.290 48.801 143.180 1.00 37.37	C
ATOM	2484 CD1 TRP B 383	31.075 48.274 145.280 1.00 37.22	
ATOM	2485 CD2 IRP B 383	33.137 47.963 144.457 1.00 37.68	
ATOM	2486 NET TRP B 383	31.107 47.058 144.650 1.00 37.31 32.354 46.839 144.130 1.00 37.64	
ATOM	2487 CE2 TRP B 383	34.470 48.015 144.037 1.00 37.73	C
ATOM	2488 CE3 TRP B 383	32.871 45.765 143.407 1.00 37.79	Č
ATOM	2489 CZ2 TRP B 383	24 077 46 051 142 322 1 00 37 20	Č
ATOM	2490 CZ3 TRP B 383	34.977 46.951 143.322 1.00 37.29 34.176 45.848 143.018 1.00 37.25	
ATOM	2491 CH2 IRP D 363	32.696 50.331 142.654 1.00 39.35	N
ATOM	2492 N LEU B 364	33.261 50.123 141.319 1.00 36.53	C
		33.201 30.123 141.319 1.00 30.33	C
	2494 C LEU B 384 2495 O LEU B 384	34.014 51.594 139.658 1.00 35.72	Ö
	2496 CB LEU B 384	32.663 48.874 140.721 1.00 35.23	C
	2497 CG LEU B 384	33.253 48.454 139.396 1.00 36.60	Č
	2497 CO LEU B 384 2498 CD1 LEU B 384	34.772 48.345 139.412 1.00 36.92	C
	2499 CD2 LEU B 384	32.657 47.092 139.012 1.00 37.73	č
	2500 N GLUB 385	32.061 52.175 140.590 1.00 36.92	N
	2500 N GLUB 385	31.952 53.382 139.753 1.00 37.16	C
	2502 C GLUB 385	33.129 54.283 140.148 1.00 36.25	c
	2502 C GLUB 385 2503 O GLUB 385	33.795 54.750 139.236 1.00 34.66	Ö
	2504 CB GLUB 385	30.637 54.128 139.876 1.00 37.88	C
	2505 CG GLU B 385	29.493 53.756 138.966 1.00 39.57	Č
	2506 CD GLUB 385	28.199 54.483 139.316 1.00 42.23	Č
	2507 OE1 GLU B 385		Ö
ATOM	2307 OET GLU D 383	27,302 34.039 140.332 1.00 42.10	Č

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ATOM	2508 OE2 GLU B 385		0
ATOM			N
		34.451 55.261 141.945 1.00 37.19	С
ATOM			C
ATOM		36.546 55.501 140.817 1.00 36.90	0
	2513 CB ILE B 386		C
		33.382 55.630 144.240 1.00 39.88	C
		35.634 56.462 143.765 1.00 36.99	C
		32.672 56.921 143.933 1.00 41.15	С
		36.060 53.423 141.602 1.00 37.58	N
ATOM	2518 CA LEU B 387	37.306 52.866 141.102 1.00 38.24	С
<b>ATOM</b>	2519 C LEUB 387		C
<b>ATOM</b>			О
<b>ATOM</b>		37.438 51.357 141.255 1.00 38.20	С
		37.692 50.790 142.649 1.00 38.34	С
ATOM	2523 CD1 LEU B 387	37.643 49.271 142.608 1.00 37.67	С
	2524 CD2 LEU B 387		С
		36.405 52.962 138.815 1.00 39.11	N
		36.503 53.166 137.381 1.00 37.80	С
<b>ATOM</b>	2527 C MET B 388	36.748 54.614 137.027 1.00 37.69	С
<b>ATOM</b>	2528 O MET B 388		О
	2529 CB MET B 388		С
<b>ATOM</b>	2530 CG MET B 388	34.931 51.198 136.866 1.00 37.83	С
<b>ATOM</b>	2531 SD MET B 388	33.953 50.509 135.536 1.00 40.19	S
<b>ATOM</b>	2532 CE MET B 388		С
	2533 N ILE B 389		N
<b>ATOM</b>	2534 CA ILE B 389	36.407 56.973 137.194 1.00 39.99	С
	2535 C ILE B 389		С
		38.556 58.002 136.800 1.00 41.50	Ο
<b>ATOM</b>	2537 CB ILE B 389	35.399 57.998 137.723 1.00 38.80	С
		35.616 59.387 137.127 1.00 38.04	C
		35.499 58.074 139.230 1.00 38.43	С
		34.371 60.249 137.198 1.00 37.00	С
		38.360 56.778 138.629 1.00 41.85	N
	2542 CA GLY B 390	39.739 57.039 139.007 1.00 43.61	С
ATOM	2543 C GLY B 390	40.671 56.515 137.914 1.00 44.49	C
	2544 O GLY B 390	41.563 57.248 137.453 1.00 44.84	О
	2545 N LEUB 391	40.437 55.247 137.542 1.00 43.58	N
	2546 CA LEUB 391	41.278 54.649 136.503 1.00 42.72	С
	2547 C LEUB 391	41.281 55.524 135.266 1.00 43.00	С
ATOM	2548 O LEUB 391	42.277 55.979 134.733 1.00 42.87	0
	2549 CB LEUB 391	40.739 53.275 136.131 1.00 42.28	C
	2550 CG LEUB 391	41.364 52.583 134.924 1.00 42.42	С
ATOM	2551 CD1 LEU B 391		С
ATOM	2552 CD2 LEU B 391	40.780 51.204 134.661 1.00 42.70	С

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ATOM		40.083 55.797 134.767 1.00 44.30	N
	2554 CA VAL B 392	39.888 56.599 133.564 1.00 44.62	С
	2555 C VAL B 392	40.696 57.890 133.661 1.00 45.80	С
	2556 O VAL B 392	41.483 58.277 132.782 1.00 46.09	0
		38.385 56.870 133.329 1.00 42.95	С
		38.164 57.928 132.274 1.00 42.03	С
		37.697 55.589 132.880 1.00 41.82	С
	2560 N TRP B 393	40.489 58.565 134.786 1.00 46.23	N
	2561 CA TRP B 393	41.156 59.836 135.033 1.00 47.70	С
	2562 C TRP B 393		С
	2563 O TRP B 393	43.349 60.532 134.370 1.00 50.15	0
	2564 CB TRP B 393	40.728 60.368 136.388 1.00 47.66	С
	2565 CG TRP B 393		C
		42.529 61.268 137.963 1.00 49.10	С
	2567 CD2 TRP B 393	41.793 62.749 136.452 1.00 49.37	С
	2568 NE1 TRP B 393	43.196 62.453 138.162 1.00 48.69	N
	2569 CE2 TRP B 393	42.762 63.374 137.260 1.00 48.40	С
	2570 CE3 TRP B 393	41.179 63.478 135.425 1.00 49.82	С
	2571 CZ2 TRP B 393	43.122 64.691 137.078 1.00 48.39	С
		41.546 64.799 135.246 1.00 49.75	С
	2573 CH2 TRP B 393	42.503 65.383 136.081 1.00 49.28	С
	2574 N ARG B 394	43.221 58.741 135.690 1.00 48.15	N
	2575 CA ARG B 394	44.665 58.624 135.677 1.00 48.22	С
	2576 C ARG B 394	45.114 58.067 134.345 1.00 49.34	C
	2577 O ARG B 394	46.307 58.107 134.051 1.00 50.97	Ο
ATOM	2578 CB ARG B 394	45.277 57.829 136.820 1.00 47.90	С
<b>ATOM</b>	2579 CG ARG B 394	44.677 56.582 137.366 1.00 46.59	С
<b>ATOM</b>	2580 CD ARG B 394	45.468 56.021 138.547 1.00 45.18	С
<b>ATOM</b>	2581 NE ARG B 394	45.074 54.602 138.668 1.00 46.07	N
<b>ATOM</b>	2582 CZ ARG B 394		
<b>ATOM</b>	2583 NH1 ARG B 394	43.142 55.189 139.769 1.00 46.63	N
<b>ATOM</b>	2584 NH2 ARG B 394		N
<b>ATOM</b>	2585 N SER B 395	44.231 57.530 133.519 1.00 50.71	N
<b>ATOM</b>	2586 CA SER B 395	44.647 56.956 132.249 1.00 51.33	С
<b>ATOM</b>	2587 C SER B 395	44.612 57.948 131.116 1.00 53.69	C <sub>i</sub>
<b>ATOM</b>	2588 O SER B 395	45.009 57.595 130.014 1.00 52.96	0
<b>ATOM</b>	2589 CB SER B 395	43.671 55.822 131.926 1.00 50.07	С
<b>ATOM</b>	2590 OG SER B 395	44.140 54.648 132.551 1.00 50.14	О
<b>ATOM</b>	2591 N MET B 396	44.095 59.141 131.377 1.00 57.28	N
	2592 CA MET B 396	43.935 60.187 130.401 1.00 60.41	С
	2593 C MET B 396	45.075 60.457 129.431 1.00 63.46	С
	2594 O MET B 396	44.857 60.432 128.205 1.00 63.38	0
	2595 CB MET B 396	43.710 61.506 131.146 1.00 60.26	C
	2596 CG MET B 396	42.519 62.275 130.599 1.00 61.44	С
ATOM	2597 SD MET B 396	41.916 63.340 131.936 1.00 63.26	S

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ATOM	2598	CE MET B 396	42.092 64.928 131.150 1.00 63.32	C
ATOM	2599	N GLUB 397	46.269 60.729 129.980 1.00 65.76	N
			47.405 61.033 129.138 1.00 68.66	C
ATOM			48.127 59.824 128.639 1.00 67.15	C
ATOM	2602		49.341 59.857 128.451 1.00 68.54	0
ATOM	2603	CB GLUB 397	48.455 61.883 129.846 1.00 74.19	C
ATOM	2604	CG GLUB 397	47.902 63.090 130.581 1.00 81.83	C
ATOM	2605	CD GLUB 397	47.274 62.607 131.891 1.00 86.58 47.662 61.462 132.279 1.00 87.97	C
		OEI GLUB 397	47.662 61.462 132.279 1.00 87.97	0
ATOM			46.420 63.332 132.488 1.00 89.52	. 0
		N HIS B 398		N
			48.211 57.461 127.941 1.00 64.09	C
		C HIS B 398		C
ATOM				0
ATOM			48.584 56.429 128.983 1.00 65.04	C
			49,573 56,912 129,992 1.00 66.53	C
			49.334 58.079 130.682 1.00 67.12	N
			50.750 56.456 130.455 1.00 67.25	C
-			50.288 58.363 131.527 1.00 68.05	С
ATOM		NE2 HIS B 398		N
		N PRO B 399		N
		CA PRO B 399		С
		C PRO B 399		C
		O PRO B 399	47,297 55.215 124.385 1.00 61.33	0
ATOM		CB PRO B 399		C
ATOM			47.011 59.217 124.246 1.00 60.94	C
			47.706 58.775 125.500 1.00 60.85	C
		N GLY B 400		N
ATOM		CA GLY B 400		С
ATOM			45.542 52.704 125.217 1.00 57.83	С
		O GLY B 400		0
		N LYS B 401	45.915 53.242 126.369 1.00 56.30	N
		CA LYS B 401	46.304 52.433 127.494 1.00 55.69	С
		C LYS B 401	45.550 52.773 128.782 1.00 53.97	С
<b>ATOM</b>	2632	O LYS B 401	44.950 53.834 128.945 1.00 53.24	0
		CB LYS B 401	47.760 52.670 127.822 1.00 58.12	С
		CG LYS B 401	48.775 52.737 126.722 1.00 61.08	С
		CD LYS B 401	49.742 51.563 126.877 1.00 64.21	С
<b>ATOM</b>	2636	CE LYS B 401	50.482 51.307 125.564 1.00 66.02	С
<b>ATOM</b>	2637	NZ LYS B 401	51.024 52.633 125.124 1.00 67.99	N
		N LEU B 402	45.640 51.805 129.691 1.00 51.90	N
		CA LEUB 402	45.012 51.988 130.990 1.00 51.47	С
		C LEU B 402	46.091 51.851 132.079 1.00 51.01	C
		O LEU B 402	46.703 50.795 132.242 1.00 50.99	0
ATOM	2642	CB LEU B 402	43.866 51.034 131.283 1.00 50.72	С

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ATOM	2643	CG LEUB 402	42.665 51.047 130.345 1.00 50.65	С
		CD1 LEU B 402	41.818 49.791 130.586 1.00 51.08	С
		CD2 LEU B 402	41.830 52.300 130.522 1.00 49.10	С
		N LEU B 403	46.285 52.928 132.827 1.00 49.42	N
		CA LEU B 403	47.230 52.971 133.906 1.00 48.91	С
		C LEU B 403	46.653 52.489 135.221 1.00 48.89	С
ATOM	2649	O LEU B 403	46.344 53.335 136.081 1.00 49.61	0
ATOM	2650	CB LEUB 403	47.635 54.452 134.090 1.00 50.09	С
<b>ATOM</b>	2651	CG LEUB 403	48.949 54.589 134.873 1.00 50.88	С
ATOM	2652	CD1 LEU B 403	50.141 54.474 133.943 1.00 50.73	С
ATOM	2653	CD2 LEU B 403	48.971 55.896 135.626 1.00 51.49	С
ATOM	2654	N PHE B 404	46.515 51.182 135.453 1.00 48.07	N
<b>ATOM</b>	2655	CA PHE B 404	45.970 50.750 136.745 1.00 48.28	С
		C PHE B 404	46.818 51.327 137.861 1.00 49.45	С
ATOM	2657	O PHE B 404	46.299 51.826 138.854 1.00 50.59	0
ATOM	2658	CB PHE B 404	45.845 49.232 136.911 1.00 47.54	С
<b>ATOM</b>	2659	CG PHE B 404	44.705 48.761 136.042 1.00 47.17	С
			44.918 48.494 134.696 1.00 47.57	С
			43.442 48.625 136.566 1.00 47.02	С
		_	43.881 48.078 133.880 1.00 47.18	С
<b>ATOM</b>		CE2 PHE B 404	42.401 48.207 135.759 1.00 47.59	С
ATOM		CZ PHE B 404	42.619 47.926 134.415 1.00 47.23	С
		N ALA B 405	48.123 51.241 137.700 1.00 51.22	N
			49.104 51.761 138.632 1.00 53.22	С
		C ALA B 405	50.194 52.524 137.898 1.00 54.37	C
		O ALA B 405	50.376 52.443 136.687 1.00 55.44	0
			49.744 50.597 139.382 1.00 52.66	C
		N PRO B 406	51.038 53.219 138.656 1.00 55.09	N
			52.179 53.966 138.148 1.00 54.47	С
			53.075 52.904 137.526 1.00 54.12	С
			53.693 53.198 136.519 1.00 56.78	0
		CB PRO B 406	52.865 54.697 139.295 1.00 53.61	C
		CG PRO B 406	51.876 54.542 140.395 1.00 53.88	C
		CD PRO B 406	50.980 53.359 140.110 1.00 54.88	C
		N ASN B 407	53.112 51.726 138.094 1.00 52.81	N
		CA ASN B 407	53.875 50.628 137.605 1.00 53.06	C
		C ASN B 407	53.019 49.505 137.050 1.00 54.38	С
		O ASN B 407	53,463 48,349 137,090 1.00 55.05	0
ATOM		CB ASN B 407	54.750 50.056 138.697 1.00 54.10	C C
		CG ASN B 407	53.941 49.244 139.687 1.00 55.16	0
		OD1 ASN B 407	52.821 49.611 140.031 1.00 56.90	N
		ND2 ASN B 407	54.492 48.136 140.145 1.00 55.04	N N
ATOM		N LEUB 408	51.825 49.796 136.536 1.00 55.00	C
ATOM		CA LEUB 408	51.037 48.720 135.898 1.00 55.25	c
ATOM	2687	C LEU B 408	50.281 49.440 134.782 1.00 55.80	C

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ATOM	2823	CD2 PHE B 425	42.031 46.381 128.907 1.00 47.63 40.983 45.815 131.396 1.00 47.70 42.833 45.916 129.923 1.00 48.04	C	
ATOM	2824	CE1 PHE B 425	40.983 45.815 131.396 1.00 47.70	С	
ATOM	2825	CE2 PHE B 425	42.833 45.916 129.923 1.00 48.04	С	
ATOM	2826	C7 PHE B 425	42.321 45.625 131.176 1.00 47.39		
ATOM	2827	N ASP B 426	37.448 48.532 126.499 1.00 49.87		
ATOM	2828	CA ASP B 426	37.056 49.426 125.412 1.00 50.42	С	
ATOM	2829	C ASP B 426	36.260 50.583 125.947 1.00 50.41	С	
ATOM	2830	O ASP B 426	36.621 51.751 125.704 1.00 50.89	0	
ATOM	2831	CB ASP B 426	36.416 48.590 124.331 1.00 53.00	С	
ATOM	2832	CG ASP B 426	37.493 48.057 123.392 1.00 55.59	С	
ATOM	2833	OD1 ASP B 426	38.621 48.596 123.480 1.00 56.98	Ο	
ATOM	2834	OD2 ASP B 426	37.224 47.143 122.584 1.00 57.24	0	
ATOM	2835	N MET B 427	35.223 50.294 126.740 1.00 49.36	N	
ATOM	2836	CA MET B 427	34.406 51.361 127.343 1.00 47.10	С	
ATOM	2837	C MET B 427	35.274 52.289 128.191 1.00 45.73	С	•
ATOM	2838	O MET B 427	35.167 53.530 128.150 1.00 43.48	0	
ATOM	2839	CB MET B 427	33.310 50.689 128.159 1.00 47.07	С	
ATOM	2840	CG MET B 427	32.326 49.996 127.228 1.00 48.35	С	•
ATOM	2841	SD MET B 427	30.954 49.295 128.150 1.00 51.41	S	
ATOM	2842	CE MET B 427	31.695 47.858 128.915 1.00 50.08	С	
ATOM	2843	N LEUB 428	36.196 51.637 128.952 1.00 43.54	N	
ATOM	2844	CA LEUB 428	37.108 52.444 129.758 1.00 41.57	С	
ATOM	2845	C LEU B 428	37.918 53.393 128.895 1.00 42.27	С	
ATOM	2846	O LEU B 428	37.993 54.612 129.123 1.00 41.21	Ο .	
<b>ATOM</b>	2847	CB LEU B 428	37.967 51.529 130.595 1.00 39.86	С	
ATOM	2848	CC I EII B 428	37 222 50 863 131 757 1 00 39 33	Ċ	
ATOM	2849	CD1 LEU B 428	38.136 49.799 132.341 1.00 39.15	С	
ATOM	2850	CD2 LEU B 428	36.829 31.864 132.828 1.00 36.37	C	
ATOM	2851	N LEUB 429	38.515 52.861 127.811 1.00 43.16	N	
ATOM	2852	CA LEU B 429	39.324 53.737 126.937 1.00 42.07	С	
ATOM	2853	C LEU B 429	38.533 54.891 126.369 1.00 41.89	, <b>C</b>	
ATOM	2854	O LEUB 429	38.920 56.061 126.439 1.00 40.64		
			40.032 52.867 125.927 1.00 41.42	C	
		CG LEUB 429	41.087 51.945 126.563 1.00 41.63	C	
		CD1 LEU B 429	41.449 50.835 125.579 1.00 43.40	<b>C</b> .	
		CD2 LEU B 429	42.326 52.705 126.967 1.00 41.22	С	
		N ALA B 430	37.351 54.571 125.841 1.00 42.23	N	
		CA ALAB 430	36.449 55.586 125.310 1.00 42.34	С	
		C ALA B 430	36.171 56.692 126.310 1.00 43.49	C	
		O ALA B 430	36.128 57.878 125.983 1.00 44.91	0	•
		CB ALAB430	35.110 54.930 125.035 1.00 42.24	C	
		N THR B 431	35.931 56.335 127.580 1.00 44.17	N	
		CA THR B 431	35.678 57.383 128.568 1.00 43.93	C	
ATOM			36.941 58.214 128.760 1.00 44.46	С	
ATOM	2867	O THR B 431	36.949 59.439 128.787 1.00 43.85	0	

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	2868 CB THR B 431	35.365 56.767 129.941 1.00 43.22	С
		34.490 55.700 129.613 1.00 44.07	0
ATOM	2870 CG2 THR B 431	34.770 57.811 130.856 1.00 42.46	С
		38.036 57.451 128.885 1.00 45.42	N
ATOM		39,336 58.071 129.093 1.00 46.40	C
ATOM		39.624 59.090 128.007 1.00 47.18	C
ATOM	2874 O SER B 432	40.081 60.200 128.226 1.00 46.93	0
ATOM	2875 CB SER B 432	40.426 57.005 129.165 1.00 46.68	C
		41.615 57.762 129.362 1.00 47.93	0
ATOM		39.322 58.696 126.779 1.00 49.00	N
ATOM	2878 CA SER B 433	39.439 59.529 125.597 1.00 50.60	С
ATOM	2879 C SER B 433	38.550 60.765 125.663 1.00 51.04	C
ATOM	2880 O SER B 433	38.936 61.913 125.493 1.00 49.73 38.933 58.601 124.478 1.00 51.44	0
ATOM	2881 CB SER B 433	38.933 58.601 124.478 1.00 51.44	C
ATOM	2882 OG SER B 433	39.347 59.183 123.261 1.00 54.59	0
		37.257 60.564 125.992 1.00 52.57	N
		36.343 61.687 126.091 1.00 53.56	C
	2885 C ARG B 434		С
	2886 O ARG B 434		O C
		34.897 61.260 126.323 1.00 54.32	C
		34.002 62.475 126.553 1.00 57.09 32.656 62.443 125.853 1.00 59.84	
ATOM	2889 CD ARG B 434	31.929 63.746 125.929 1.00 62.03	N N
ATOM	2890 NE ARG B 434	32.361 64.759 125.146 1.00 62.85	C
		33.422 64.480 124.363 1.00 64.15	N
ATOM ATOM		31.824 65.968 125.103 1.00 61.67	N
	2894 N PHE B 435		N
ATOM		37.988 63.060 129.258 1.00 56.24	C
ATOM	2896 C PHE B 435	39.122 63.878 128.661 1.00 57.90	c
ATOM		39.213 65.071 128.914 1.00 57.34	Ö
ATOM		38.418 62.337 130.527 1.00 56.05	C
	2899 CG PHE B 435	37.308 62.036 131.502 1.00 56.15	C .
	2900 CD1 PHE B 435	36.024 62.524 131.369 1.00 55.57	C
	2901 CD2 PHE B 435	37.568 61.227 132.593 1.00 56.19	Ċ
	2902 CE1 PHE B 435	35.037 62.232 132.264 1.00 55.28	C
	2903 CE2 PHE B 435	36.594 60.905 133.516 1.00 56.05	С
	2904 CZ PHE B 435	35.316 61.417 133.338 1.00 56.32	С
	2905 N ARG B 436	39.955 63.231 127.854 1.00 60.28	N
	2906 CA ARG B 436	41.058 63.905 127.192 1.00 62.39	С
<b>ATOM</b>	2907 C ARG B 436	40.479 65.002 126.321 1.00 63.40	С
ATOM	2908 O ARG B 436	40.774 66.177 126.463 1.00 64.03	Ο
<b>ATOM</b>	2909 CB ARG B 436	41.829 62.929 126.314 1.00 63.83	С
	2910 CG ARG B 436	43.304 63.231 126.193 1.00 66.34	С
	2911 CD ARG B 436	44.026 62.204 125.336 1.00 69.23	С
ATOM	2912 NE ARG B 436	43.917 60.836 125.853 1.00 71.66	N

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ATOM	2958 CA GLY B 442	41.451 67.852 138.380 1.00 58.59	С
ATOM	2959 C GLY B 442	40.381 68.371 139.311 1.00 57.45	С
ATOM	2960 O GLY B 442	39.750 67.550 139.971 1.00 57.67	Ο
ATOM	2961 N GLUB 443	40.110 69.665 139.394 1.00 57.46	N
<b>ATOM</b>	2962 CA GLUB 443	39.071 70.172 140.290 1.00 58.76	С
ATOM	2963 C GLUB 443	37.701 69.598 139.853 1.00 56.56	C
ATOM	2964 O GLUB 443	36.801 69.336 140.659 1.00 55.98	0
ATOM	2965 CB GLUB 443	38.915 71.685 140.392 1.00 61.69	C
ATOM	2966 CG GLUB 443	40.077 72.578 140.705 1.00 65.54	C C
ATOM	2967 CD GLUB 443 2968 OE1 GLUB 443	41.234 72.324 139.750 1.00 69.36 41.018 72.218 138.513 1.00 70.43	0
ATOM	2969 OE2 GLU B 443	42.375 72.210 140.277 1.00 71.96	0
ATOM ATOM		37.557 69.444 138.539 1.00 53.20	N
ATOM	2971 CA GLUB 444	36.342 68.887 137.981 1.00 50.57	C
ATOM	2972 C GLU B 444	36.286 67.415 138.361 1.00 49.12	c
	2973 O GLUB 444	35.270 66.955 138.881 1.00 49.11	Ö
	2974 CB GLUB 444	36.350 69.031 136.465 1.00 50.33	С
	2975 CG GLUB 444	35.989 70.466 136.085 1.00 49.89	С
ATOM		36.187 70.701 134.602 1.00 50.08	С
ATOM	2977 OE1 GLU B 444	37.163 70.127 134.046 1.00 49.93	0
ATOM	2978 OE2 GLUB 444	35.324 71.458 134.107 1.00 50.00	О
ATOM	2979 N PHE B 445	37.398 66.720 138.123 1.00 47.04	N
ATOM	2980 CA PHE B 445	37.485 65.299 138.458 1.00 45.59	C
ATOM	2981 C PHE B 445	36.995 64.993 139.867 1.00 46.10	С
ATOM	2982 O PHE B 445	36.101 64.205 140.163 1.00 46.63	O C
ATOM	2983 CB PHE B 445 2984 CG PHE B 445	38.919 64.814 138.315 1.00 43.27 39.145 63.452 138.876 1.00 42.65	C
ATOM ATOM		38.452 62.370 138.401 1.00 43.72	C
ATOM		40.046 63.227 139.881 1.00 43.37	Č
ATOM		38.644 61.098 138.909 1.00 44.67	Č
ATOM	2988 CE2 PHE B 445	40.284 61.979 140.419 1.00 43.66	C
ATOM		39.574 60.907 139.917 1.00 44.59	С
	2990 N VAL B 446	37.590 65.656 140.833 1.00 46.31	N
ATOM	2991 CA VAL B 446	37.277 65.532 142.254 1.00 46.33	С
<b>ATOM</b>	2992 C VAL B 446	35.810 65.787 142.543 1.00 47.52	С
	2993 O VAL B 446	35.184 65.166 143.431 1.00 48.08	О
	2994 CB VAL B 446	38.311 66.442 142.934 1.00 45.14	C
	2995 CG1 VAL B 446	37.743 67.475 143.832 1.00 45.02	C
	2996 CG2 VAL B 446	39.302 65.572 143.699 1.00 45.97	C
	2997 N CYS B 447	35.158 66.685 141.809 1.00 47.38	N
	2998 CA CYS B 447	33.755 66.952 142.040 1.00 48.88	C C
	2999 C CYS B 447 3000 O CYS B 447	32.865 65.818 141.558 1.00 49.14 31.941 65.374 142.235 1.00 49.68	0
	3000 O CYS B 447 3001 CB CYS B 447	33.375 68.225 141.275 1.00 50.13	C
	3001 CB C13 B 447	33.720 69.719 142.194 1.00 53.53	S
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ATOM	3003	N LEUB 448	33.122 65.336 140.341 1.00 48.95	Ν
ATOM		CA LEU B 448	32.344 64.260 139.734 1.00 47.16	С
ATOM		C LEU B 448	32.437 63.023 140.618 1.00 46.56	С
ATOM		O LEUB 448	31.432 62.376 140.924 1.00 47.61	0
ATOM		CB LEU B 448	32.865 63.902 138.361 1.00 47.65	С
ATOM		CG LEUB 448	32.616 64.881 137.213 1.00 48.16	С
ATOM		CDI LEU B 448	33.430 64.435 135.992 1.00 48.65	С
		CD2 LEU B 448	31.135 64.937 136.890 1.00 47.17	С
<b>ATOM</b>	3011	N LYS B 449	33.650 62.740 141.087 1.00 44.57	N
ATOM	3012	CA LYS B 449	33.830 61.590 141.963 1.00 43.44	С
ATOM		C LYS B 449	32.912 61.728 143.151 1.00 43.26	С
ATOM		O LYS B 449	32.262 60.740 143.539 1.00 44.55	0
		CB LYS B 449	35.304 61.464 142.272 1.00 44.12	C
		CG LYS B 449	35.798 60.032 142.426 1.00 44.36	C
		CD LYS B 449	36.782 60.041 143.569 1.00 45.90	C
		CE LYS B 449	38.197 60.360 143.103 1.00 46.74	C
		NZ LYS B 449	39.081 60.103 144.303 1.00 48.51	N
ATOM		N SER B 450	32.765 62.899 143.767 1.00 42.43	N C
		CA SER B 450	31.846 62.976 144.909 1.00 42.81 30.399 62.836 144.484 1.00 41.70	c
ATOM		C SER B 450 O SER B 450	29.594 62.261 145.208 1.00 42.04	0
ATOM		CB SER B 450	31.905 64.329 145.633 1.00 44.22	C
ATOM ATOM		OG SER B 450	33.285 64.483 145.953 1.00 48.34	Ö
ATOM		N ILE B 451	30.067 63.392 143.318 1.00 40.21	N
		CA ILE B 451	28.689 63.295 142.852 1.00 38.74	C
ATOM		C ILE B 451	28,361 61.816 142.756 1.00 38.58	C
ATOM		O ILE B 451	27.305 61.378 143.211 1.00 37.33	Ö
ATOM		CB ILE B 451	28.571 64.007 141.514 1.00 39.81	С
			28.772 65.508 141.765 1.00 40.80	С
			27,239 63.690 140.853 1.00 39.99	С
<b>ATOM</b>	3033	CD1 ILE B 451	28.421 66.370 140.544 1.00 42.17	·C
ATOM	3034	N ILE B 452	29.284 61.035 142.170 1.00 38.63	N
		CA ILE B 452	29.082 59.592 142.020 1.00 37.62	С
		C ILE B 452	28.825 58.938 143.373 1.00 38.09	C
		O ILE B 452	27.889 58.162 143.541 1.00 37.47	0
		CB ILE B 452	30.270 58.895 141.326 1.00 36.64	C
		CG1 ILE B 452	30.469 59.451 139.926 1.00 36.43	C
		CG2 ILE B 452	30.041 57.381 141.292 1.00 36.66	C
		CD1 ILE B 452	31.347 58.695 138.958 1.00 35.50	C
		N LEUB 453	29.658 59.254 144.362 1.00 38.77	N
		CA LEUB 453	29,499 58.683 145.683 1.00 39.54	C C
		C LEUB 453	28.130 59.031 146.243 1.00 40.27 27.508 58.168 146.829 1.00 41.50	0
		O LEUB 453	30.559 59.195 146.693 1.00 38.52	C
		CB LEU B 453 CG LEU B 453	30.293 58.818 148.163 1.00 36.48	C
ATOM	JU4/	CG LEU D 433	JU, 273 JO, 010 170, 103 1,00 JU,40	C

14.751 58.678 155.954 1.00104.27

15.196 58.536 154.585 1.00 99.91

14.861 59.789 153.786 1.00 96.52 15.661 60.257 152.986 1.00 96.33

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ATOM 3137 N SER B 468 ATOM 3138 CA SER B 468

ATOM 3139 C SER B 468

ATOM 3140 O SER B 468

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ATOM	3141 CB SER B 468	14.518 57.369 153.865 1.00100.33	C
ATOM	3142 OG SER B 468	14.946 56.142 154.419 1.00101.36 13.669 60.334 154.008 1.00 92.58	0
ATOM	3143 N LEUB 469	13.669 60.334 154.008 1.00 92.58	N
ATOM	3144 CA LEUB 469	13.240 61.536 153.297 1.00 89.00	С
		14.176 62.663 153.687 1.00 86.59	C
ATOM	3146 O LEUB 469	14.526 63.522 152.886 1.00 86.06	0
ATOM	3147 CB LEUB 469	11.775 61.857 153.578 1.00 89.46 14.614 62.658 154.934 1.00 84.75	С
ATOM	3151 N GLUB 470	14.614 62.658 154.934 1.00 84.75	N
ATOM	3132 CA GLU B 470	13.55 US.080 133.409 1.00 65.61	С
<b>ATOM</b>	3153 C GLUB 470	16.940 63.374 154.870 1.00 79,82	С
ATOM	3154 O GLUB 470	17.699 64.245 154.462 1.00 78.99	0
<b>ATOM</b>	3155 CB GLUB 470	15.408 63.750 156.913 1.00 88.01 16.703 63.787 157.705 1.00 93.53	С
<b>ATOM</b>	3156 CG GLUB 470	16.703 63.787 157.705 1.00 93.53	С
<b>ATOM</b>	3157 CD GLUB 470	16.434 63.541 159.185 1.00 97.16	С
ATOM	3158 OE1 GLU B 470	15.314 63.053 159.516 1.00 98.71	0
ATOM	3159 OE2 GLU B 470	17.365 63.849 159.982 1.00 99.17	0
<b>ATOM</b>	3160 N GLUB 471	17.323 62.106 154.807 1.00 75.78 18.593 61.660 154.266 1.00 71.86	N
ATOM	3161 CA GLUB 471	18.593 61.660 154.266 1.00 71.86	С
ATOM	3162 C GLUB 471	18.605 62.021 152.775 1.00 70.49	С
		19.582 62.544 152.244 1.00 71.13	0
ATOM	3164 CB GLUB 471	18 795 60 156 154 404 1 00 70 33	С
ATOM	3165 CG GLUB 471	18.983 59.604 155 781 1.00 69.51	C
ATOM	3166 CD GLUB 471	18.983 59.604 155.781 1.00 69.51 20.401 59.447 156.253 1.00 69.90	C
ATOM	3167 OE1 GLUB 471	21.123 58.551 155.784 1.00 69.90	O
		20.888 60.204 157.125 1.00 70.61	Ō
		17.512 61.755 152.064 1.00 68.23	N
		17.443 62.094 150.661 1.00 66.98	C
ATOM	3171 C LYS B 472	17.599 63.591 150.478 1.00 65.63	C
ATOM	3172 O LYS B 472	18.392 63.964 149.607 1.00 65.62	Ö
		16.170 61.590 150.011 1.00 68.62	C
		16.125 60.081 149.849 1.00 71.13	Č
	3175 CD LYS B 472	15.015 59.682 148.893 1.00 74.04	Č
	3176 CE LYS B 472	14.408 58.333 149.248 1.00 76.38	Č
	3177 NZ LYS B 472	15.152 57.157 148.664 1.00 77.87	N
	3178 N ASP B 473	16.920 64.440 151.237 1.00 64.78	N
	3179 CA ASP B 473	17.082 65.877 151.034 1.00 65.36	C
	3180 C ASP B 473	18.516 66.332 151.232 1.00 62.76	c
	3181 O ASP B 473	19.109 67.035 150.430 1.00 63.80	Ö
	3182 CB ASP B 473	16.291 66.752 152.000 1.00 69.33	C
	3183 CG ASP B 473	14.816 66.470 151.832 1.00 73.90	C
	3184 OD1 ASP B 473	14.441 65.701 150.904 1.00 76.03	O
	3185 OD2 ASP B 473	14.069 67.050 152.657 1.00 76.73	0
	3186 N HIS B 474	19.072 65.908 152.354 1.00 59.23	N
	3187 CA HIS B 474	20.449 66.243 152.659 1.00 56.40	C
	3188 C HIS B 474	21.328 65.998 151.428 1.00 55.19	c
WI OIM	2100 € ДВВ 4/4	21.320 UJ.770 IJI.420 I.UU JJ.19	C

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ATOM	3189	O HIS B 474	22.045 66.881 150.947 1.00 53.51	0
		CB HIS B 474	20.887 65.360 153.835 1.00 55.62	С
		CG HIS B 474	22.279 65.818 154.180 1.00 56.07	С
			22.540 67.145 154.498 1.00 55.48	N
ATOM	3193	CD2 HIS B 474	23.435 65.111 154.203 1.00 56.58	С
		CE1 HIS B 474	23.843 67.220 154.730 1.00 56.88	С
		NE2 HIS B 474	24.410 66.017 154.559 1.00 57.47	N
		N ILE B 475	21.250 64.758 150.917 1.00 54.03	N
		CA ILE B 475	22.003 64.377 149.746 1.00 53.42	С
		C ILE B 475	21.668 65.281 148.572 1.00 53.75	C
		O ILE B 475	22.569 65.802 147.901 1.00 52.81	0
		CB ILE B 475	21.753 62.918 149.374 1.00 53.33	С
		CG1 ILE B 475	22.378 62.047 150.462 1.00 53.70	C C
		CG2 ILE B 475	22.370 62.593 148.021 1.00 53.57 22.291 60.573 150.105 1.00 54.14	C
		CD1 ILE B 475	20.391 65.533 148.302 1.00 54.79	N
		N HIS B 476 CA HIS B 476	20.391 63.333 146.302 1.00 34.79 20.092 66.414 147.169 1.00 57.16	C
		C HIS B 476	20.729 67.776 147.357 1.00 58.28	c
		O HIS B 476	21.293 68.396 146.440 1.00 58.61	Ö
			18.596 66.470 146.957 1.00 59.37	Č
		CG HIS B 476		Č
			18.745 64.600 145.267 1.00 62.78	N
		CD2 HIS B 476	16.989 64.450 146.584 1.00 61.95	С
		CE1 HIS B 476	18.057 63.517 144.922 1.00 63.31	C
		NE2 HIS B 476	16.995 63.403 145.701 1.00 62.29	N
		N ARG B-477	20.681 68.281 148.587 1.00 59.16	N
ATOM	3215	CA ARG B 477	21.236 69.547 148.986 1.00 58.98	С
		C ARG B 477	22.726 69.681 148.710 1.00 57.17	С
		O ARG B 477	23.164 70.678 148.124 1.00 56.93	0
		CB ARG B 477	21.033 69.701 150.492 1.00 62.77	C
		CG ARG B 477	20.678 71.151 150.807 1.00 69.05	С
		CD ARGB 477	19.157 71.257 150.564 1.00 74.67	C
ATOM	3221	NE ARGB4//	18.517 70.405 151.574 1.00 79.86 18.429 70.786 152.859 1.00 82.73	N C
			18.429 70.786 132.839 1.00 82.73	N
		NH2 ARG B 477		N
		N VAL B 478	23,494 68,680 149,141 1.00 54.36	N
		CA VAL B 478	24.943 68.675 148.939 1.00 52.49	Ċ
		C VAL B 478	25.235 68.604 147.450 1.00 52.18	C
		O VAL B 478	26.104 69.239 146.842 1.00 51.94	Ö.
		CB VAL B 478	25.543 67.480 149.693 1.00 52.54	C
		CG1 VAL B 478	27.053 67.386 149.590 1.00 52.18	C
		CG2 VAL B 478		С
		N LEUB 479	24.407 67.803 146.763 1.00 51.49	N
		CA LEU B 479	24.513 67.646 145.311 1.00 49.86	С

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ATOM	3234	C LEU B 479		С
ATOM		O LEU B 479		0
ATOM			23.496 66.630 144.787 1.00 46.59	С
ATOM		CG LEUB 479		С
ATOM	3238	CD1 LEU B 479		С
ATOM		CD2 LEU B 479		С
ATOM		N ASP B 480		N
ATOM			23.365 71.196 144.568 1.00 52.25	С
ATOM	3242	C ASP B 480	24.633 71.994 144.842 1.00 52.37	С
ATOM		O ASP B 480		0
ATOM	3244	CB ASP B 480	22.148 71.963 145.047 1.00 53.28	С
ATOM	3245	CG ASP B 480	20.835 71.318 144.638 1.00 54.67	С
ATOM	3246	OD1 ASP B 480	20.799 70.546 143.657 1.00 55.26	0
ATOM	3247	OD2 ASP B 480	19.791 71.559 145.291 1.00 55.41	0
		N LYS B 481		N
ATOM	3249	CA LYS B 481	26.357 72.608 146.440 1.00 54.79	С
ATOM		C LYS B 481		С
			28.165 73.015 144.955 1.00 55.38	0
			26.743 72.364 147.889 1.00 58.10	С
			27.789 73.346 148.394 1.00 62.90	С
ATOM	3254	CD LYS B 481	27.145 74.541 149.106 1.00 66.84	С
ATOM	3255	CE LYS B 481	27.999 75.805 149.020 1.00 69.39	С
ATOM	3256	NZ LYS B 481	29.024 75.782 147.919 1.00 71.15	N
ATOM	3257	N ILE B 482	27.646 70.855 145.320 1.00 52.58	N
ATOM	3258	CA ILE B 482	28.705 70.401 144.407 1.00 50.25	С
ATOM	3259	C ILE B 482	28.406 70.935 143.020 1.00 49.16	С
ATOM	3260	O ILE B 482	29.350 71.353 142.339 1.00 49.20	Ο
ATOM	3261	CB ILE B 482	28.917 68.898 144.435 1.00 49.88	С
ATOM	3262	CG1 ILE B 482	29.455 68.527 145.825 1.00 50.32	С
ATOM	3263	CG2 ILE B 482	29.934 68.446 143.417 1.00 49.96	С
ATOM		CD1 ILE B 482	28.834 67.247 146.349 1.00 51.02	С
ATOM		N THR B 483		N
ATOM			26.874 71.594 141.288 1.00 49.74	С
		C THR B 483		С
		O THR B 483		0
		CB THR B 483		С
ATOM	3270	OG1 THR B 483	25.050 70.188 140.912 1.00 49.10	0
		CG2 THR B 483	25.071 72.316 139.717 1.00 49.01	С
		N ASP B 484	27.017 73.834 142.213 1.00 51.19	N
		CA ASP B 484	27.476 75.218 142.294 1.00 50.56	С
		C ASP B 484	29.002 75.268 142.245 1.00 50.46	С
ATOM			29.605 76.073 141.522 1.00 51.67	Ο
ATOM	3276	CB ASP B 484	27.001 75.898 143.558 1.00 50.97	С
		CG ASP B 484		С
ATOM	3278	OD1 ASP B 484	24.853 75.982 142.497 1.00 53.11	Ο
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183/371 24.940 76.307 144.717 1.00 53.76 ATOM 3279 OD2 ASP B 484 0 ATOM 3280 N THR B 485 29.694 74.386 142.956 1.00 49.24 N ATOM 3281 CA THR B 485 31.154 74.396 142.907 1.00 49.60 C C ATOM 3282 C THR B 485 31.680 74.196 141.495 1.00 50.42 ATOM 3283 O THR B 485 32.684 74.791 141.087 1.00 50.51 O 31.664 73.271 143.835 1.00 48.97 C ATOM 3284 CB THR B 485 ATOM 3285 OG1 THR B 485 30.967 73.451 145.080 1.00 47.88 0 33.176 73.286 143.960 1.00 47.44 C ATOM 3286 CG2 THR B 485 31.002 73.328 140.741 1.00 51.30 ATOM 3287 N LEUB 486 N 31.433 73.036 139.368 1.00 51.82 C ATOM 3288 CA LEUB 486 ATOM 3289 C LEU B 486 31.339 74.277 138.479 1.00 52.24 C 32,257 74,683 137,774 1.00 50.69 0 ATOM 3290 O LEUB 486 ATOM 3291 CB LEUB 486 30.573 71.907 138.761 1.00 49.64 C 31.218 70.532 138.888 1.00 48.31 C ATOM 3292 CG LEUB 486 ATOM 3293 CD1 LEU B 486 30.237 69.504 138.358 1.00 48.07 C 32,555 70.536 138.164 1.00 47.39 C ATOM 3294 CD2 LEU B 486 ATOM 3295 N ILE B 487 30.147 74.897 138.557 1.00 53.50 N ATOM 3296 CA ILE B 487 29.921 76.092 137.754 1.00 55.16 C ATOM 3297 C ILE B 487 30.953 77.157 138.134 1.00 57.21 C ATOM 3298 O ILE B 487 31.609 77.809 137.322 1.00 57.31 0 ATOM 3299 CB ILE B 487 28.510 76.631 137.978 1.00 54.14 C 27.457 75.695 137.432 1.00 54.26 C ATOM 3300 CG1 ILE B 487 C ATOM 3301 CG2 ILE B 487 28.458 77.994 137.316 1.00 55.14 C 27.219 75.771 135.943 1.00 54.81 ATOM 3302 CD1 ILE B 487 31.105 77.327 139.446 1.00 58.96 N ATOM 3303 N HIS B 488 C ATOM 3304 CA HIS B 488 32.052 78.277 139.982 1.00 60.55 ATOM 3305 C HIS B 488 33.385 78.041 139.302 1.00 60.12 33,987 78,945 138,743 1.00 61.16 ATOM 3306 O HIS B 488 0 ATOM 3307 CB HIS B 488 32.201 78.053 141.481 1.00 63.98 C ATOM 3308 CG HIS B 488 33.356 78.861 142.005 1.00 67.76 ATOM 3309 ND1 HIS B 488 33.313 80.239 142.060 1.00 68.99 N C 34.573 78.457 142.475 1.00 69.21 ATOM 3310 CD2 HIS B 488 ATOM 3311 CE1 HIS B 488 34.481 80.641 142.565 1.00 70.75 Ċ 35.266 79.590 142.831 1.00 70.44 N ATOM 3312 NE2 HIS B 488 33,870 76,808 139,343 1.00 59.86 N ATOM 3313 N LEU B 489 35.140 76.503 138.700 1.00 60.03 C ATOM 3314 CA LEU B 489 35.214 76.966 137.242 1.00 60.16 ATOM 3315 C LEU B 489 C 36.162 77.570 136.755 1.00 58.98 ATOM 3316 O LEUB 489 0 C ATOM 3317 CB LEU B 489 35.311 74.975 138.755 1.00 58.86 35.797 74.471 140.096 1.00 59.40 C ATOM 3318 CG LEUB 489 35.741 72.942 140.083 1.00 60.90 ATOM 3319 CD1 LEU B 489 C

37.209 74.937 140.395 1.00 59.49

34.193 76.643 136.465 1.00 61.21

34.095 78.425 134.725 1.00 62.90

34.106 76.937 135.052 1.00 62.35

ATOM 3320 CD2 LEU B 489

ATOM 3321 N MET B 490

ATOM 3322 CA MET B 490 ATOM 3323 C MET B 490

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ATOM	3324 O MET B 490	34.731 78.867 133 768 1.00 62.67	О
ATOM	3325 CB MET B 490	32.807 76.321 134 - 00 1.00 62.53	С
ATOM	3326 CG MET B 490	33.018 74.922 133 939 1.00 62.79	С
ATOM	3327 SD MET B 490	31.400 74.130 133.827 1.00 64.70	S
ATOM	3328 CE MET B 490	31.840 72.442 134.233 1.00 63.89	С
ATOM	3329 N ALA B 491	33.336 79.163 135.541 1.00 63.19	N
ATOM	3330 CA ALA B 491	33.245 80.608 135.353 1.00 63.40	С
ATOM	3331 C ALA B 491	34.665 81.115 135.583 1.00 63.75	С
		35.219 81.807 134.739 1.00 63.44	Ο
		32.252 81.242 136.296 1.00 63.10	С
ATOM	3334 N LYS B 492	35.288 80.683 136.678 1.00 64.63	N
ATOM	3335 CA LYS B 492	36.662 81.082 136.954 1.00 66.16	С
ATOM	3336 C LYS B 492	37.545 80.773 135.765 1.00 66.57	С
		38.458 81.559 135.514 1.00 68.67	0
		37.235 80.489 138.236 1.00 66.65	С
		37.346 79.758 134.952 1.00 67.06	N
ATOM	3344 CA ALA B 493	38.181 79.515 133.784 1.00 68.05	C
ATOM	3345 C ALA B 493	38.181 79.515 133.784 1.00 68.05 37.649 80.371 132.632 1.00 69.31	С
		38.043 80.265 131.472 1.00 70.45	0
		38.217 78.061 133.355 1.00 67.81	С
		36.705 81.254 132.897 1.00 69.82	N
ATOM	3349 CA GLY B 494	36.112 82.145 131.941 1.00 70.15	С
ATOM	3350 C GLY B 494	35.391 81.444 130.819 1.00 70.48	С
		35.767 81.599 129.655 1.00 72.21	0
ATOM	3352 N LEUB 495	34.359 80.656 131.074 1.00 70.34	N
<b>ATOM</b>	3353 CA LEUB 495	33.646 80.047 129.944 1.00 69.20	С
		32.365 80.888 129.907 1.00 68.78	С
<b>ATOM</b>	3355 O LEUB 495	31.928 81.311 130.977 1.00 67.73	Ο
		33.255 78.597 130.088 1.00 68.95	С
<b>ATOM</b>	3357 CG LEUB 495	34.298 77.596 130.577 1.00 69.01	С
		33.750 76.182 130.417 1.00 69.36	
<b>ATOM</b>	3359 CD2 LEU B 495	35.598 77.732 129.809 1.00 69.12	С
<b>ATOM</b>	3360 N THR B 496	31.817 81.101 128.735 1.00 69.23	N
<b>ATOM</b>	3361 CA THR B 496	30.574 81.867 128.685 1.00 70.03	С
<b>ATOM</b>	3362 C THR B 496	29,554 81.192 129.572 1.00 70.46	С
<b>ATOM</b>	3363 O THR B 496	29.688 80.016 129.897 1.00 71.40	Ο
	3364 CB THR B 496	29.987 81.709 127.275 1.00 70.86	С
ATOM	3365 OG1 THR B 496	30.999 82.069 126.332 1.00 72.15	Ο
<b>ATOM</b>	3366 CG2 THR B 496	28.731 82.529 127.084 1.00 72.22	С
<b>ATOM</b>	3367 N LEUB 497	28.476 81.872 129.917 1.00 71.30	N
ATOM		27.413 81.282 130.717 1.00 71.94	С
<b>ATOM</b>	3369 C LEUB 497	26.818 80.089 129.961 1.00 72.66	С
<b>ATOM</b>	3370 O LEUB 497	26.362 79.078 130.509 1.00 72.74	0
<b>ATOM</b>	3371 CB LEUB 497	26.361 82.336 130.938 1.00 73.14	С
<b>ATOM</b>	3372 CG LEU B 497	25.737 82.520 132.308 1.00 75.05	С

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3386	C GLN B 499		С
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3404	C HIS B 501		C
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3417	N GLN B 502	26.669 73.995 129.009 1.00 53.45	N
	3373 3374 3375 3376 3377 3378 3379 3380 3381 3382 3383 3384 3385 3386 3387 3393 3394 3395 3396 3397 3398 3396 3397 3400 3401 3402 3403 3404 3405 3406 3407 3408 3410 3411 3412 3413 3416	3382 OE1 GLN B 498 3383 NE2 GLN B 498 3384 N GLN B 499 3385 CA GLN B 499 3386 C GLN B 499 3387 O GLN B 499 3388 CB GLN B 499 3389 CG GLN B 499 3390 CD GLN B 499 3391 OE1 GLN B 499 3392 NE2 GLN B 499 3393 N GLN B 500 3394 CA GLN B 500 3395 C GLN B 500 3396 O GLN B 500 3397 CB GLN B 500 3398 CG GLN B 500 3399 CD GLN B 500 3400 OE1 GLN B 500 3401 NE2 GLN B 500 3401 NE2 GLN B 500	185

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ATOM	3418	CA GLN B 502	26.940 72.871 128.127 1.00 52.90	С
		C GLN B 502	27.942 71.918 128.772 1.00 52.22	С
		O GLN B 502	27.647 70.721 128.922 1.00 51.61	Ο
		CB GLN B 502	27.422 73.419 126.787 1.00 54.22	С
ATOM		CG GLN B 502	26.373 74.342 126.184 1.00 55.11	С
ATOM		CD GLN B 502	26.499 74.615 124.704 1.00 54.93	С
		OE1 GLN B 502	27.619 74.599 124.169 1.00 55.67	Ο
		NE2 GLN B 502	25,343 74.862 124.089 1.00 53.79	N
		N ARG B 503	29.108 72.384 129.218 1.00 50.84	N
		CA ARG B 503	30.092 71.560 129.898 1.00 48.49	С
		C ARG B 503	29.463 70.800 131.069 1.00 48.40	С
		O ARG B 503	29.729 69.604 131.216 1.00 49.87	0
ATOM		CB ARG B 503	31,217 72,421 130,495 1,00 47,02	C
ATOM		CG ARG B 503	32,435 71,558 130,785 1,00 47,10	С
ATOM		CD ARG B 503	33.700 72.366 130.968 1.00 45.82	С
		NE ARG B 503	34,788 71,588 131,542 1.00 45.26	N
		CZ ARG B 503	35.665 70.918 130.815 1.00 46.26	С
		NH1 ARG B 503	35.568 70.910 129.493 1.00 46.31	N
		NH2 ARG B 503	36.669 '70.235 131.366 1.00 47.52	N
		N LEUB 504	28.644 71.462 131.888 1.00 46.45	N
		CA LEU B 504	28.023 70.802 133.014 1.00 45.17	С
		C LEU B 504	27.339 69.548 132.495 1.00 46.22	С
ATOM		O LEU B 504	27.695 68.426 132.869 1.00 47.23	0
ATOM	3441	CB LEU B 504	27.017 71.705 133.720 1.00 43.90	С
		CG LEU B 504	26.422 71.152 135.018 1.00 43.02	С
ATOM	3443	CD1 LEU B 504	27.484 70.796 136.035 1.00 42.09	С
ATOM	3444	CD2 LEU B 504	25.434 72.161 135.603 1.00 42.49	С
ATOM	3445	N ALA B 505	26.384 69.771 131.586 1.00 46.57	N
ATOM	3446	CA ALA B 505	25.639 68.658 130.986 1.00 45.30	С
ATOM	3447	C ALA B 505	26.622 67.677 130.371 1.00 46.91	С
ATOM	3448	O ALA B 505	26.518 66.469 130.660 1.00 48.20	O
<b>ATOM</b>	3449	CB ALA B 505	24.658 69.248 130.021 1.00 44.08	С
<b>ATOM</b>	3450	N GLN B 506	27.629 68.077 129.585 1.00 47.50	N
<b>ATOM</b>	3451	CA GLN B 506	28.566 67.094 129.051 1.00 47.74	C
<b>ATOM</b>	3452	C GLN B 506	29.206 66.326 130.190 1.00 48.34	С
<b>ATOM</b>	3453	O GLN B 506	29.273 65.098 130.031 1.00 50.56	0
<b>ATOM</b>	3454	CB GLN B 506	29.642 67.637 128.122 1.00 48.83	C
<b>ATOM</b>	3455	CG AGLN B 506	29.324 68.944 127.440 0.50 49.79	C
<b>ATOM</b>	3456	CG BGLN B 506	29.073 68.052 126.764 0.50 49.57	С
<b>ATOM</b>	3457	CD AGLN B 506	30.244 69.417 126.351 0.50 50.30	С
<b>ATOM</b>	3458	CD BGLN B 506	28.599 66.920 125.870 0.50 49.56	С
<b>ATOM</b>	3459	OE1AGLN B 506		0
ATOM	3460	OE1BGLN B 506	29.020 65.770 126.068 0.50 50.14	0
ATOM	3461	NE2AGLN B 506	29.672 69.881 125.241 0.50 50.69	N
<b>ATOM</b>	3462	NE2BGLN B 506	27.744 67.233 124.896 0.50 48.23	N

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ATOM	3463	N LEUB 507	29.637 66.940 131.278 1.00 48.08	N
ATOM	3464	CA LEU B 507	30.249 66.175 132.359 1.00 48.18	C
ATOM	3465	C LEU B 507	29.274 65.201 132.999 1.00 47.50	С
ATOM	3466	O LEU B 507	29.611 64.010 133.075 1.00 49.50	Ο
<b>ATOM</b>	3467	CB LEU B 507	30.821 67.077 133.452 1.00 49.39	С
ATOM	3468	CG LEU B 507	32.048 67.900 133.026 1.00 50.17	С
ATOM	3469	CD1 LEU B 507	32.468 68.844 134.135 1.00 49.83	С
ATOM	3470	CD2 LEU B 507	33.163 66.965 132.590 1.00 50.59	С
ATOM	3471	N LEUB 508	28.108 65.661 133.416 1.00 45.18	N
ATOM	3472	CA LEU B 508	27.146 64.743 134.024 1.00 44.33	С
ATOM	3473	C LEU B 508	26.695 63.653 133.076 1.00 44.72	С
ATOM	3474	O LEU B 508	26.456 62.520 133.573 1.00 46.18	Ο
ATOM	3475	CB LEU B 508	25.969 65.562 134.561 1.00 43.86	С
ATOM	3476	CG LEU B 508	26.418 66.604 135.595 1.00 44.31	С
ATOM	3477	CD1 LEU B 508	25.304 67.481 136.094 1.00 44.65	С
ATOM	3478	CD2 LEU B 508	27.001 65.893 136.814 1.00 46.31	С
ATOM	3479	N LEUB 509	26.631 63.860 131.740 1.00 42.70	N
ATOM	3480	CA LEU B 509	26.188 62.738 130.907 1.00 41.76	С
<b>ATOM</b>	3481	C LEU B 509	27.166 61.568 130.901 1.00 42.73	C
<b>ATOM</b>	3482	O LEU B 509	26.750 60.415 130.677 1.00 42.98	Ο
ATOM	3483	CB LEU B 509	25.771 63.111 129.500 1.00 39.78	С
ATOM	3484	CG LEU B 509	24.498 63.933 129.331 1.00 39.38	С
ATOM	3485	CD1 LEU B 509	24.376 64.378 127.887 1.00 39.53	С
ATOM	3486	CD2 LEU B 509	23.261 63.183 129.768 1.00 38.89	С
ATOM	3487	N ILE B 510	28.452 61.794 131.175 1.00 42.74	N
<b>ATOM</b>	3488	CA ILEB 510	29.430 60.702 131.201 1.00 42.35	С
		C ILEB510	29.081 59.803 132.385 1.00 41.76	С
ATOM	3490	O ILE B 510	29,280 58,577 132,334 1.00 41.62	О
ATOM	3491	CB ILE B 510	30.874 61.227 131.277 1.00 42.40	С
<b>ATOM</b>	3492	CGI ILE B 510	31.414 61.613 129.902 1.00 43.54	С
ATOM	3493	CG2 ILE B 510	31.861 60.190 131.777 1.00 42.50	С
ATOM	3494	CD1 ILE B 510	32.106 62.960 129.894 1.00 45.42	С
ATOM	3495	N LEUB 511	28.525 60.389 133.451 1.00 40.66	N
<b>ATOM</b>	3496	CA LEUB 511	28.170 59.585 134.616 1.00 42.25	С
<b>ATOM</b>	3497	C LEU B 511	27.297 58.398 134.249 1.00 42.82	С
ATOM	3498	O LEU B 511	27.463 57.267 134.735 1.00 43.36	О
<b>ATOM</b>	3499	CB LEUB 511	27.601 60.448 135.730 1.00 42.09	С
ATOM	3500	CG LEUB 511	28.535 61.542 136.285 1.00 41.35	С
ATOM	3501	CD1 LEU B 511	27.865 62.131 137.519 1.00 41.68	C
		CD2 LEU B 511	29.923 61.032 136.646 1.00 39.19	С
		N SER B 512	26.357 58.553 133.328 1.00 42.90	N
ATOM	3504	CA SER B 512	25.559 57.466 132.826 1.00 42.26	С
		C SER B 512	26.408 56.302 132.306 1.00 42.66	C
		O SER B 512	26.211 55.124 132.655 1.00 43.46	О
<b>ATOM</b>	3507	CB SER B 512	24.841 57.983 131.565 1.00 43.15	С

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		189/371	
ATOM	3553 N MET B 517	29.102 50.984 132.602 1.00 40.61	N
	3554 CA MET B 517	30.341 50.227 132.704 1.00 41.77	С
	3555 C MET B 517	30.489 49.440 133.998 1.00 42.00	С
<b>ATOM</b>	3556 O MET B 517	30.894 48.283 134.051 1.00 41.42	Ο
	3557 CB MET B 517	31.525 51.198 132.723 1.00 42.99	С
	3558 CG MET B 517	32.313 51.172 131.425 1.00 45.13	C
ATOM	3559 SD MET B 517	33.516 52.536 131.360 1.00 46.85	S
ATOM	3560 CE MET B 517	32.400 53.916 131.339 1.00 48.12	С
	3561 N SER B 518	30.140 50.131 135.092 1.00 42.51	N
ATOM	3562 CA SER B 518	30.228 49.515 136.415 1.00 42.93	C
ATOM	3563 C SER B 518	29.290 48.320 136.489 1.00 42.97	C
ATOM	3564 O SER B 518	29.653 47.306 137.096 1.00 42.01	0
ATOM	3565 CB SER B 518	29.912 50.557 137.469 1.00 43.94	C
	3566 OG SER B 518	29.230 50.022 138.586 1.00 45.24 28.112 48.471 135.868 1.00 43.73	O N
	3567 N ASN B 519 3568 CA ASN B 519	27.136 47.379 135.882 1.00 45.19	C
ATOM		27.767 46.200 135.165 1.00 46.03	c
ATOM			Ö
	3571 CB ASN B 519		Č
	3572 CG ASN B 519	24.993 48.638 136.263 1.00 49.48	Č
	3573 OD1 ASN B 519	25.089 48.397 137.490 1.00 51.53	0
ATOM		24,208 49.617 135,798 1.00 49.53	N
ATOM	3575 N LYS B 520	28.347 46.392 133.986 1.00 46.49	N
<b>ATOM</b>	3576 CA LYS B 520	29.000 45.306 133.272 1.00 46.97	С
ATOM	3577 C LYS B 520	30.174 44.793 134.099 1.00 46.60	C
ATOM	3578 O LYS B 520	30.331 43.573 134.240 1.00 47.54	0
ATOM	3579 CB LYS B 520	29.523 45.785 131.920 1.00 48.14	C
ATOM		28.432 46.661 131.298 1.00 50.82	C
	3581 CD LYS B 520	27.655 45.791 130.346 1.00 54.22	C
	3582 CE LYS B 520	26.190 45.599 130.698 1.00 56.72	C
	3583 NZ LYS B 520	25.690 44.401 129.918 1.00 58.52	N N
ATOM	3584 N GLY B 521	30.957 45.705 134.659 1.00 44.61 32.043 45.239 135.494 1.00 45.54	C
	3585 CA GLY B 521 3586 C GLY B 521	31.596 44.324 136.628 1.00 46.50	c
	3587 O GLY B 521	32.325 43.332 136.830 1.00 46.54	ŏ
	3588 N MET B 522	30.503 44.577 137.382 1.00 46.75	N
	3589 CA MET B 522	30.195 43.644 138.449 1.00 47.80	C
	3590 C MET B 522	29.807 42.299 137.819 1.00 48.57	С
		30.240 41.253 138.299 1.00 49.08	0
	3592 CB MET B 522	29.062 43.838 139.401 1.00 48.14	С
<b>ATOM</b>	3593 CG MET B 522	28.578 45.083 140.019 1.00 48.74	С
	3594 SD MET B 522	29.593 45.740 141.330 1.00 50.47	S
	3595 CE MET B 522	30.303 44.236 141.989 1.00 48.09	С
	3596 N GLUB 523	28.988 42.406 136.780 1.00 50.12	N
ATOM	3597 CA GLUB 523	28.571 41.169 136.107 1.00 51.27	С

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			190/371	
ATOM	3598	C GLU B 523	29,801 40,335 135,793 1.00 48.34	С
<b>ATOM</b>	3599		29.842 39.152 136.111 1.00 48.80	Ο
<b>ATOM</b>	3600	CB GLU B 523	27.693 41.477 134.926 1.00 56.32	С
<b>ATOM</b>	3601	CG GLU B 523	26.222 41.586 135.253 1.00 63.90	С
<b>ATOM</b>	3602	CD GLU B 523	25.669 40.410 136.046 1.00 69.58	С
<b>ATOM</b>	3603	OE1 GLU B 523	26.274 39.292 136.084 1.00 72.07	0
<b>ATOM</b>	3604	OE2 GLU B 523	24.573 40.579 136.664 1.00 72.34	0
<b>ATOM</b>	3605	N HIS B 524	30.835 40.904 135.228 1.00 45.16	N
<b>ATOM</b>	3606	CA HIS B 524	32.042 40.187 134.925 1.00 44.63	С
<b>ATOM</b>	3607	C HIS B 524	32.786 39.694 136.136 1.00 45.63	С
<b>ATOM</b>	3608	O HIS B 524	33.174 38.530 136.210 1.00 46.13	0
<b>ATOM</b>	3609	CB HIS B 524	32.941 41.153 134.131 1.00 44.39	С
<b>ATOM</b>	3610	CG HIS B 524	34.264 40.554 133.809 1.00 45.05	С
<b>ATOM</b>	3611	ND1 HIS B 524	35.340 40.624 134.677 1.00 46.06	N
<b>ATOM</b>	3612	CD2 HIS B 524	34.689 39.871 132.727 1.00 45.55	С
<b>ATOM</b>	3613	CE1 HIS B 524	36.379 40.011 134.130 1.00 46.99	С
<b>ATOM</b>	3614	NE2 HIS B 524	36.014 39.538 132.934 1.00 46.65	N
<b>ATOM</b>		N LEUB 525	33.040 40.541 137.136 1.00 47.40	N
<b>ATOM</b>		CA LEU B 525	33.838 40.173 138.305 1.00 48.66	С
<b>ATOM</b>	3617	C LEU B 525	33.186 38.970 138.973 1.00 51.45	С
<b>ATOM</b>		O LEUB 525	33.801 38.061 139.503 1.00 51.39	0
		CB LEU B 525	34.009 41.328 139.283 1.00 47.23	С
		CG LEUB 525	34.669 40.941 140.610 1.00 46.40	С
		CD1 LEU B 525	36.099 40.533 140.321 1.00 46.02	C
ATOM		CD2 LEU B 525	34.591 42.051 141.634 1.00 46.06	С
ATOM		N TYR B 526	31.860 39.006 138.936 1.00 54.54	N
ATOM		CA TYR B 526	31.029 37.963 139.465 1.00 58.05	С
ATOM		C TYR B 526	31.236 36.681 138.674 1.00 59.70	C
ATOM	3626		31.383 35.663 139.357 1.00 60.78	0
ATOM		CB TYR B 526	29.591 38.447 139.352 1.00 60.78	C
ATOM		CG TYR B 526	28.713 37.388 139.962 1.00 64.37	C
		CD1 TYR B 526	28.504 37.370 141.319 1.00 66.32	C
		CD2 TYR B 526	28.117 36.424 139.178 1.00 66.84	C
		CE1 TYR B 526	27.700 36.427 141.916 1.00 68.78	C
		CE2 TYR B 526	27.300 35.457 139.738 1.00 69.50	С
		CZ TYR B 526	27.112 35.477 141.106 1.00 70.89	C
		OH TYR B 526	26.313 34.509 141.697 1.00 74.25	0
		N SER B 527	31.261 36.673 137.336 1.00 60.47	N
		CA SER B 527	31.498 35.385 136.667 1.00 61.49	C
		C SER B 527	32.948 35.014 136.945 1.00 61.49	C
		O SER B 527	33.157 33.877 137.371 1.00 62.15	0
		CB SER B 527	31.192 35.377 135.188 1.00 62.44	C
		OG SER B 527	31.689 36.588 134.634 1.00 63.98	0
		N MET B 528	33.911 35.911 136.843 1.00 61.64	N
ATOM	3642	CA MET B 528	35.281 35.555 137.196 1.00 63.8°	С

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ΔΤΩΜ	3643	C MET B 528	35,329 34,828 138,542 1.00 64.80	С
		O MET B 528	36.067 33.868 138.753 1.00 63.49	Ö
		CB MET B 528	36.167 36.800 137.243 1.00 64.77	С
		CG MET B 528	36.878 37.227 135.984 1.00 65.29	С
<b>ATOM</b>	3647	SD MET B 528	37.201 35.912 134.760 1.00 66.35	S
<b>ATOM</b>	3648	CE MET B 528	35.670 36.008 133.820 1.00 65.10	С
		N LYS B 529	34.553 35.264 139.522 1.00 67.52	N
		CA LYS B 529	34.492 34.654 140.833 1.00 70.80	С
		C LYS B 529	33.860 33.273 140.754 1.00 72.85	C
		O LYS B 529	34.298 32.357 141.450 1.00 73.96	0
			33.705 35.538 141.795 1.00 71.14	C
			32.734 34.819 142.692 1.00 72.73	C
			32.855 35.292 144.119 1.00 75.27	C C
		CE LYS B 529	31.706 34.773 144.975 1.00 77.62 30.380 34.816 144.286 1.00 78.57	N
		N CYS B 530	32.815 33.113 139.964 1.00 75.23	N
			32.150 31.817 139.833 1.00 78.47	C
		C CYS B 530	33.059 30.823 139.165 1.00 80.04	c
		O CYS B 530	33.123 29.653 139.549 1.00 81.22	Ö
			30.800 32.058 139.165 1.00 79.44	C
			29.756 32.972 140.357 0.50 80.86	S
		SG BCYS B 530	29.435 31.171 139.942 0.50 81.98	S
		N LYS B 531	33.878 31.218 138.207 1.00 81.81	N
		CA LYS B 531	34.846 30.378 137.528 1.00 83.72	С
		C LYS B 531		C
			37.009 29.407 138.089 1.00 85.56	0
ATOM	3669	CB LYS B 531	35.405 31.112 136.302 1.00 84.17	C
			34,640 30.945 135.014 1.00 85.13	C C
			33.167 31.305 135.153 1.00 86.04	N
			36.050 30.578 139.651 1.00 86.77 37.099 30.391 140.629 1.00 88.41	C
			38.429 30.832 140.066 1.00 87.48	c
		O ASN B 532	39.358 30.052 139.939 1.00 88.95	Ö
		CB ASN B 532	37.128 28.922 141.046 1.00 91.42	C
		CG ASN B 532	35.880 28.573 141.848 1.00 94.45	C
			35.454 29.327 142.741 1.00 95.85	0
		ND2 ASN B 532	35.297 27.420 141.516 1.00 95.63	N
<b>ATOM</b>	3682	N VAL B 533	38.555 32.084 139.686 1.00 86.02	N
		CA VAL B 533	39.753 32.676 139.116 1.00 84.42	С
		C VAL B 533	40.242 33.838 139.982 1.00 84.06	C
		O VAL B 533	41.369 34.303 140.067 1.00 84.64	0
		CB VAL B 533	39.383 33.246 137.730 1.00 83.89	C
			40.659 33.683 137.031 1.00 84.42	C
			38.598 32.275 136.875 1.00 83.22 39.311 34.417 140.708 1.00 83.35	C N
AIUM	७०४५	N VAL B 534	34.41/ 140.706 1.00 83.33	14

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			193/371	
ATOM	3739	N LEU B 540	36.688 43.219 148.933 1.00 53.90	N
		CA LEUB 540	36.181 43.177 147.572 1.00 52.79	С
		C LEU B 540	34.995 42.215 147.482 1.00 53.01	C
		O LEU B 540	33.997 42.532 146.834 1.00 51.76	0
		CB LEU B 540	37.305 42.784 146.604 1.00 52.02	С
		CG LEUB 540	36.956 42,739 145.109 1.00 50.85	С
		CDI LEU B 540	36.882 44.150 144.556 1.00 50.14	С
		CD2 LEU B 540	37.918 41.898 144.288 1.00 49.04	С
		N LEUB 541	35.009 41.061 148.168 1.00 54.06	N
		CA LEU B 541	33.851 40.167 148.078 1.00 55.51	С
		C LEU B 541	32.655 40.800 148.757 1.00 54.97	С
		O LEU B 541		0
			34.142 38.728 148.519 1.00 57.67	С
		CG LEU B 541	35.260 38.143 147.614 1.00 61.07	С
		CD1 LEU B 541	35.784 36.793 148.069 1.00 62.23	С
ATOM	3754	CD2 LEU B 541	34.853 38.060 146.141 1.00 61.20	С
ATOM	3755	N GLU B 542	32.959 41.581 149.781 1.00 54.14	N
ATOM	3756	CA GLUB 542	31.900 42.280 150.518 1.00 53.44	С
<b>ATOM</b>	3757	C GLU B 542	31.240 43'.265 149.573 1.00 52.31	С
	3758		30.027 43.175 149.439 1.00 53.50	Ο
		CB GLUB 542	32.503 42.961 151.720 1.00 54.11	С
		CG GLUB 542	31.596 43.714 152.660 1.00 55.33	C
		CD GLUB 542	32.440 44.275 153.805 1.00 56.53	C
		OE1 GLU B 542	33.437 43.602 154.207 1.00 56.98	0
		OE2 GLU B 542	32.128 45.369 154.319 1.00 56.39	0
		N MET B 543	31.971 44.138 148.901 1.00 50.59	N
		CA MET B 543	31.349 45.101 148.005 1.00 49.97	C
		C MET B 543	30.635 44.411 146.876 1.00 50.80	C
		O MET B 543	29.540 44.816 146.450 1.00 52.14	O C
		CB MET B 543	32.413 46.070 147.501 1.00 50.12 33.138 46.730 148.686 1.00 50.55	C
		CG MET B 543 SD MET B 543	32.069 48.020 149.371 1.00 50.36	S
ATOM ATOM		CE MET B 543	31.905 47.356 151.033 1.00 52.76	C
		N LEU B 544	31.229 43.343 146.348 1.00 51.11	N
		CA LEU B 544	30.559 42.599 145.275 1.00 51.10	Ċ
		C LEU B 544	29.248 42.015 145.783 1.00 52.28	c
		O LEU B 544	28.286 42.170 145.059 1.00 50.33	Ö
		CB LEU B 544	31.466 41.517 144.722 1.00 50.23	C
		CG LEU B 544	30.929 40.494 143.735 1.00 49.60	Č
		CD1 LEU B 544	30.393 41.090 142.446 1.00 48.96	C
		CD2 LEU B 544	32.032 39.505 143.390 1.00 49.82	Č
ATOM		N ASP B 545	29.195 41.388 146.960 1.00 56.16	N
		CA ASP B 545	27.967 40.810 147.477 1.00 60.23	С
		C ASP B 545	26.867 41.826 147.692 1.00 60.49	C
ATOM			25.711 41.499 147.422 1.00 61.09	0

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ATOM 3784 CB ASP B 5	45 28.103 40.031 148.779 1.00 64.79	С
ATOM 3785 CG ASP B 5		С
ATOM 3786 OD1 ASP B		Ο
ATOM 3787 OD2 ASP B		0
ATOM 3788 N ALA B 54		N
ATOM 3789 CA ALAB 5		C
ATOM 3790 C ALAB 54		C
ATOM 3791 O ALAB 54		0
ATOM 3792 CB ALABS		C
ATOM 3793 N HIS B 54		N
ATOM 3794 CA HIS B 54		C C
ATOM 3795 C HIS B 54' ATOM 3796 O HIS B 54'		0
ATOM 3797 CB HIS B 54		C
ATOM 3797 CB HIS B 54		C
ATOM 3798 CO 1115 B 5		N
ATOM 3800 CD2 HIS B 5		C
ATOM 3801 CE1 HIS B 5		
ATOM 3802 NE2 HIS B 5		
ATOM 3803 N ARG B 54		N
ATOM 3804 CA ARG B 5		С
ATOM 3805 C ARG B 54	48 22.972 40.425 145.078 1.00 85.03	С
ATOM 3806 O ARG B 54	48 22.876 41.170 146.088 1.00 85.76	Ο
ATOM 3807 CB ARG B 5		<b>C</b> .
ATOM 3808 CG ARG B 5		С
ATOM 3809 CD ARGB		C
ATOM 3810 NE ARG B 5		,
ATOM 3811 CZ ARG B 5		
	548 26.679 41.608 140.013 1.00 97.08	
	548 24.853 40.355 139.434 1.00 97.27	N
TER 3814 ARG B 548	COO 40 77C 47 424 120 452 1 00 25 74	C
	600 40.756 47.434 139.452 1.00 35.74 600 41.286 48.562 140.064 1.00 38.16	C
HETATM 3816 C2 EST B HETATM 3817 C3 EST B		C C
HETATM 3818 O3 EST B		0
HETATM 3819 C4 EST B		č
HETATM 3820 C5 EST B		č
HETATM 3821 C6 EST B		Č
HETATM 3822 C7 EST B		Č
HETATM 3823 C8 EST B		С
HETATM 3824 C9 EST B	600 39.261 46.343 137.787 1.00 34.78	С
HETATM 3825 C10 EST B	600 39.838 47.566 138.419 1.00 35.26	С
HETATM 3826 C11 EST B	600 39.049 45.234 138.797 1.00 34.27	С
HETATM 3827 C12 EST B		С
HETATM 3828 C13 EST B	600 37.350 44.218 137.357 1.00 34.33	С

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ITET ATT 4 2020 C14 EST P 6		С
HETATM 3829 C14 EST B 60		C
HETATM 3830 C15 EST B 60		Č
HETATM 3831 C16 EST B 60		
HETATM 3832 C17 EST B 6		
HETATM 3833 O17 EST B 6		0
HETATM 3834 C18 EST B 6		C
ATOM 3835 N SER C 305		N
ATOM 3836 CA SER C 305	4.469 36.963 108.991 1.00 89.00	C
ATOM 3837 C SER C 305	3.303 37.261 108.070 1.00 88.50	C
ATOM 3838 O SER C 305		0
ATOM 3839 CB SER C 305	5.742 36.644 108.192 1.00 88.54	С
ATOM 3840 OG SER C 305	6.028 37.662 107.253 1.00 87.89	Ο
ATOM 3841 N LEU C 306	2.873 38.521 108.031 1.00 88.30	N
ATOM 3842 CA LEU C 306	5 1.813 38.932 107.102 1.00 87.75	С
ATOM 3843 C LEU C 306		С
	1.494 37.623 105.105 1.00 86.96	Ο
	1.643 40.449 107.031 1.00 87.75	С
ATOM 3849 N ALA C 307		N
ATOM 3850 CA ALA C 30		С
ATOM 3851 C ALA C 307		C
	2.787 36.700 102.691 1.00 81.74	Ö
	7 5.499 38.153 104.101 1.00 83.87	C
ATOM 3054 N. LELLC 308	3.741 35.897 104.578 1.00 80.64	N
ATOM 3855 CA LEUC 308	3.313 34.528 104.349 1.00 80.56	Ċ
		c
ATOM 3856 C LEU C 308		Ö
ATOM 3857 O LEU C 308	1.451 33.090 104.129 1.00 81.28	C
ATOM 3858 CB LEU C 300	3 4.088 33.638 105.326 1.00 80.74 5 606 33.703 105 314 1.00 81.07	č
ATOM 3859 CG LEU C 300	3 5.606 33.702 105.214 1.00 81.07	C
ATOM 3860 CDI LEU C 30	8 6.233 32.474 105.868 1.00 81.84 8 6.072 33.806 103.771 1.00 81.43	C
		N
ATOM 3862 N SER C 309		C
ATOM 3863 CA SER C 309		
ATOM 3864 C SER C 309		С
ATOM 3865 O SER C 309		0
ATOM 3866 CB SER C 309		C
ATOM 3867 OG SER C 309		0
ATOM 3868 N LEU C 310		N
ATOM 3869 CA LEU C 310		С
ATOM 3870 C LEU C 310		С
ATOM 3871 O LEU C 310		0
ATOM 3872 CB LEU C 310	-0.896 38.740 101.649 1.00 73.31	С
ATOM 3873 CG LEU C 310	0 -0.133 39.482 102.740 1.00 72.27	С
ATOM 3874 CD1 LEU C 31	0 1.312 39.565 102.299 1.00 72.68	С
ATOM 3875 CD2 LEU C 31		C
ATOM 3876 N THR C 311		N

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ATOM	3877 CA THR C 311	-2.995 36.006 98.906 1.00 70.70	С
		-2.290 36.693 97.760 1.00 69.86	C
		-2.027 37.901 97.909 1.00 69.35	0
ATOM	3880 CB THR C 311	-4.525 35.958 98.804 1.00 70.54	С
ATOM	3881 OG1 THR C 311	-5.119 37.248 98.625 1.00 70.13	0
		-5.108 35.381 100.078 1.00 69.62	С
		-2.027 36.051 96.633 1.00 69.24	N
ATOM	3884 CA ALA C 312	-1.352 36.731 95.535 1.00 69.20	С
		-1.994 38.096 95.309 1.00 70.12	С
		-1.276 39.088 95.102 1.00 69.29	0
		-1.319 35.905 94.278 1.00 68.74	С
ATOM	3888 N ASP C 313	-3.336 38.147 95.357 1.00 71.47	N
<b>ATOM</b>	3889 CA ASP C 313	-3.987 39.441 95.163 1.00 72.61	С
<b>ATOM</b>	3890 C ASP C 313	-3.987 39.441 95.163 1.00 <b>72.</b> 61 -3.647 40.479 96.208 1.00 <b>70.88</b>	С
ATOM	3891 O ASP C 313	-3.370 41.605 95.797 1.00 70.30	0
		-5.493 39.237 95.037 1.00 76.00	С
ATOM	3893 CG ASP C 313	-5.719 38.770 93.609 1.00 <b>7</b> 9.09	C ·
ATOM	3894 OD1 ASP C 313	-5.291 39.457 92.663 1.00 80.25	0
ATOM	3895 OD2 ASP C 313	-6.310 37.698 93.443 1.00 81.73	0
		-3.619 40.161 97.488 1.00 69.54	N
		-3.275 41.129 98.517 1.00 69.05	C
ATOM	3898 C GLN C 314	-1.827 41.588 98.406 1.00 67.22	C
ATOM	3899 O GLN C 314	-1.555 42.776 98.566 1.00 67.37	0
ATOM	3900 CB GLN C 314	-3.461 40.533 99.904 1.00 71.68 -4.663 39.606 99.946 1.00 73.75	C
ATOM	3901 CG GLN C 314	-4.663 39.606 99.946 1.00 73.73	C C
		-4.941 39.149 101.358 1.00 75.13	0
		-4.588 38.039 101.724 1.00 76.64 -5.561 40.049 102.105 1.00 75.55	N
		-0.942 40.636 98.123 1.00 64.44	N
		0.470 40.910 97.899 1.00 60.68	C
		0.626 41.972 96.811 1.00 57.71	c
	3908 O MET C 315	1.238 43.010 96.977 1.00 55.57	Ö
	3909 CB MET C 315	1.140 39.614 97.448 1.00 61.06	C
	3910 CG MET C 315	2.650 39.635 97.262 1.00 61.75	C
	3911 SD MET C 315	3.583 39.449 98.818 1.00 60.96	S
	3912 CE MET C 315	4.383 41.044 98.814 1.00 61.10	C
	3913 N VAL C 316	0.044 41.766 95.642 1.00 56.70	N
	3914 CA VAL C 316	0.158 42.714 94.558 1.00 57.51	С
	3915 C VAL C 316	-0.261 44.121 94.967 1.00 59.23	С
ATOM	3916 O VAL C 316	0.397 45.117 94.654 1.00 59.22	Ο
	3917 CB VAL C 316	-0.679 42.341 93.326 1.00 56.92	С
	3918 CG1 VAL C 316	-0.569 43.429 92.272 1.00 56.72	С
	3919 CG2 VAL C 316	-0.201 41.056 92.696 1.00 57.50	С
	3920 N SER C 317	-1.408 44.225 95.634 1.00 60.46	N
ATOM	3921 CA SER C 317	-1.945 45.518 96.051 1.00 60.81	С

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ATOM	4012	CA SER C 329	14.325 67.186 88.873 1.00 68.05	С
ATOM	4013	C SER C 329	14.324 68.663 89.244 1.00 70.45	С
<b>ATOM</b>		O SER C 329		О
<b>ATOM</b>	4015	CB SER C 329	15.044 67.000 87.545 1.00 66.88	C
<b>ATOM</b>	4016	OG SER C 329	16.260 67.726 87.721 1.00 67.32	О
<b>ATOM</b>	4017	N GLU C 330	15.292 69.079 90.029 1.00 75.28	N
<b>ATOM</b>	4018	CA GLU C 330	15.486 70.451 90.466 1.00 79.72	С
<b>ATOM</b>	4019	C GLU C 330	15.752 71.335 89.247 1.00 80.73	С
ATOM	4020	O GLU C 330	16.490 71.033 88.312 1.00 81.64	О
ATOM	4021	CB GLU C 330	16.659 70.570 91.435 1.00 83.87	С
ATOM	4022	CG GLU C 330	17.883 71.352 90.984 1.00 88.78	С
ATOM	4023	CD GLU C 330	19.152 70.582 90.643 1.00 91.78	С
ATOM	4024	OE1 GLU C 330	19.923 70.181 91.569 1.00 93.23	0
<b>ATOM</b>	4025	OE2 GLU C 330	19.404 70.377 89.422 1.00 92.87	0
			24.571 71.818 80.367 1.00 86.34	N
			24.988 70.495 80.814 1.00 85.91	С
			26.498 70.301 80.720 1.00 84.19	С
			27.064 70.525 79.646 1.00 85.85	О
ATOM			24.383 69.350 79.978 1.00 87.18	С
ATOM			23.005 68.970 80.445 1.00 88.47	C
ATOM			22.650 69.084 81.778 1.00 88.68	С
			22.068 68.507 79.534 1.00 89.03	С
		CE1 PHE C 337		С
<b>ATOM</b>			20.795 68.160 79.942 1.00 89.22	C
ATOM			20.454 68.283 81.275 1.00 89.44	С
			27.095 69.868 81.803 1.00 80.55	N
ATOM			28.533 69.626 81.747 1.00 77.95	С
ATOM		C SER C 338		C
ATOM	4040		27.886 68.188 83.475 1.00 75.98	0
ATOM			29.228 70.829 82.347 1.00 78.52	C
			28.558 71.186 83.554 1.00 78.56	0
			29.821 67.656 82.395 1.00 73.78	N
			30.025 66.490 83.270 1.00 72.51	C
		C GLU C 339	29.556 66.874 84.677 1.00 71.03	C
		O GLU C 339	28.611 66.294 85.215 1.00 71.03	0
		CB GLU C 339	31.473 66.090 83.172 1.00 72.67	C
		CG GLU C 339	32.133 65.356 84.319 1.00 73.25	C
		CD GLU C 339	33.182 64.454 83.684 1.00 74.49	C
		OE1 GLU C 339	32.762 63.725 82.754 1.00 74.89	0
		OE2 GLU C 339	34.357 64.515 84.104 1.00 75.34	0
		N ALA C 340	30.147 67.886 85.304 1.00 68.89	N
		CA ALA C 340	29.747 68.302 86.619 1.00 67.05	C
		C ALA C 340	28.288 68.694 86.720 1.00 66.84	C
		O ALA C 340	27.647 68.263 87.697 1.00 68.55	0
ATOM	4056	CB ALA C 340	30.586 69.468 87.090 1.00 67.09	С

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		201/371	
ATOM	4102 O THR C 347	21.850 62.428 93.704 1.00 47.00	O
ATOM		24.621 62.957 91.764 1.00 46.71	C
ATOM		25.412 61.774 91.987 1.00 47.34	0
	4105 CG2 THR C 347	24.855 64.108 92.685 1.00 45.43	С
ATOM	4106 N ASN C 348	21.741 64.272 92.536 1.00 48.38	N
ATOM	4107 CA ASN C 348	20.800 64.933 93.432 1.00 48.80	С
ATOM	4108 C ASN C 348	19.478 64.160 93.443 1.00 47.26	С
ATOM	4109 O ASN C 348	18.850 63.828 94.448 1.00 46.97	Ο
ATOM	4110 CB ASN C 348	20.589 66.367 92.932 1.00 51.67	С
ATOM	4111 CG ASN C 348	19.510 67.096 93.727 1.00 55.80	С
<b>ATOM</b>	4112 OD1 ASN C 348	18.292 67.162 93.409 1.00 56.91	0
<b>ATOM</b>	4113 ND2 ASN C 348	20.009 67.668 94.842 1.00 56.64	N
	4114 N LEU C 349	18.996 63.846 92.246 1.00 45.48	N
	4115 CA LEU C 349	17.730 63.135 92.094 1.00 43.91	С
	4116 C LEU C 349	17.843 61.824 92.848 1.00 42.97	C
	4117 O LEU C 349	16.938 61.492 93.603 1.00 42.67	0
	4118 CB LEU C 349		C
ATOM		16.113 62.256 90.280 1.00 45.28	C
ATOM		14.890 63.005 90.815 1.00 44.98	C
	4121 CD2 LEU C 349	15.924 61.981 88.802 1.00 45.98	C
	4122 N ALA C 350	18.925 61.069 92.685 1.00 42.54	N
ATOM		19.170 59.789 93.329 1.00 41.93	C
	4124 C ALA C 350	19.145 59.965 94.846 1.00 42.66	C
	4125 O ALA C 350	18.382 59.288 95.534 1.00 42.32	O C
	4126 CB ALA C 350	20.519 59.214 92.915 1.00 41.05 19.924 60.909 95.377 1.00 42.85	N
ATOM ATOM		19.891 61.156 96.801 1.00 44.92	C
ATOM		18.473 61.409 97.333 1.00 46.20	c
ATOM		18.134 61.037 98.479 1.00 46.87	0
ATOM		20.806 62.330 97.121 1.00 47.28	C
ATOM		20.808 62.552 98.629 1.00 49.76	Č
	4133 OD1 ASP C 351	21.507 61.847 99.383 1.00 49.99	o
	4134 OD2 ASP C 351	20.076 63.475 99.055 1.00 51.97	Ö
	4135 N ARG C 352	17.580 62.055 96.578 1.00 45.35	N
	4136 CA ARG C 352	16,230 62,286 97,039 1,00 44,90	С
	4137 C ARG C 352	15.377 61.039 96.994 1.00 45.67	C
	4138 O ARG C 352	14,604 60.740 97.920 1.00 46.34	0
	4139 CB ARG C 352	15.622 63.384 96.190 1.00 45.66	С
ATOM	4140 CG ARG C 352	16.211 64.727 96.599 1.00 47.97	С
	4141 CD ARG C 352	15.095 65.784 96.368 1.00 49.73	С
ATOM	4142 NE ARG C 352	15.270 66.120 94.954 1.00 51.59	N
ATOM	4143 CZ ARG C 352	14.259 66.180 94.076 1.00 52.43	С
ATOM	4144 NH1 ARG C 352	13.012 65.962 94.496 1.00 50.90	N
ATOM	4145 NH2 ARG C 352	14.668 66.482 92.828 1.00 52.24	N
ATOM	4146 N GLU C 353	15.480 60.234 95.928 1.00 45.42	N

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ATOM	4147	CA GLU C 353	14.681 59.005 95.829 1.00 44.09	С
ATOM	4148	C GLU C 353	15.048 57.996 96.931 1.00 43.54	С
ATOM	4149		14.249 57.145 97.354 1.00 41.61	0
ATOM	4150	CB GLU C 353	14.925 58.352 94.479 1.00 43.55	С
ATOM	4151	CG GLU C 353	14.829 59.283 93.288 1.00 44.01	С
ATOM		CD GLU C 353	14.774 58.522 91.971 1.00 44.71	С
ATOM		OE1 GLU C 353	13.863 57.703 91.769 1.00 44.74	0
ATOM	4154	OE2 GLU C 353	15.652 58.718 91.111 1.00 45.16	0
		N LEUC354	16.297 58.121 97.413 1.00 42.25	N
ATOM		CA LEU C 354	16.817 57.236 98.424 1.00 42.36	С
ATOM		C LEU C 354	15.967 57.327 99.669 1.00 43.23	С
ATOM	4158	O LEU C 354	15.622 56.324 100.303 1.00 44.20	Ο
ATOM	4159	CB LEU C 354	18.300 57.512 98.701 1.00 41.72	С
ATOM	4160	CG LEU C 354	19.142 56.685 97.709 1.00 41.03	С
<b>ATOM</b>	4161	CD1 LEU C 354	20.499 57.306 97.552 1.00 41.57	С
<b>ATOM</b>	4162	CD2 LEU C 354	19.154 55.273 98.236 1.00 41.51	С
ATOM	4163	N VAL C 355	15.617 58.560 99.994 1.00 43.50	N
ATOM	4164	CA VAL C 355	14.766 58.766 101.172 1.00 43.54	С
ATOM		C VAL C 355		С
ATOM			13.044 57.168 101.749 1.00 44.67	О
ATOM	4167	CB VAL C 355	14.536 60.278 101.340 1.00 42.48	С
<b>ATOM</b>	4168	CG1 VAL C 355		C
ATOM		CG2 VAL C 355		C
ATOM		N HIS C 356		N
ATOM			11.514 57.552 99.623 1.00 45.02	С
		C HIS C 356		C
ATOM		O HIS C 356		O
ATOM			10.881 58.057 98.313 1.00 48.88	C
ATOM			10.545 59.504 98.508 1.00 51.53	C
		ND1 HIS C 356	9.269 59.940 98.714 1.00 52.82	N
=		CD2 HIS C 356		C
ATOM		CE1 HIS C 356	9.287 61.255 98.886 1.00 53.87	C
		NE2 HIS C 356	10.534 61.686 98.805 1.00 54.36	N
		N MET C 357	12.893 55.662 99.024 1.00 44.54	N
		CA MET C 357	13.210 54.233 98.928 1.00 43.62	, C
		C MET C 357	13.141 53.532 100.274 1.00 42.21	C
		O MET C 357	12.466 52.525 100.393 1.00 42.85	0
		CB MET C 357	14.574 53.907 98.327 1.00 43.25	C
		CG MET C 357	14.636 52.406 97.985 1.00 42.60	C
		SD MET C 357	16.349 52.075 97.453 1.00 42.35	S
		CE MET C 357	16.261 52.824 95.831 1.00 43.46	C
		N ILE C 358	13.834 54.096 101.243 1.00 40.42	N
		CA ILE C 358	13.815 53.539 102.582 1.00 39.96	C
		C ILE C 358	12.394 53.337 103.074 1.00 41.38	С
ATOM	4191	O ILE C 358	12.056 52.287 103.607 1.00 41.84	О

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			203/371	
ATOM	4192	CB ILE C 358	14.587 54.473 103.522 1.00 37.30	С
		CG1 ILE C 358	16.020 54.488 103.073 1.00 37.04	С
ATOM		CG2 ILE C 358	14.503 54.006 104.933 1.00 37.30	С
		CD1 ILE C 358	16.901 55.392 103.869 1.00 38.43	С
ATOM	4196	N ASN C 359	11.533 54.324 102.909 1.00 43.86	N
ATOM	4197	CA ASN C 359	10.146 54.230 103.335 1.00 46.73	С
ATOM	4198	C ASN C 359	9.476 53.068 102.650 1.00 46.07	Ç
ATOM		O ASN C 359	8.928 52.164 103.263 1.00 47.05	О
ATOM		CB ASN C 359	9.407 55.532 103.002 1.00 52.10	C
ATOM		CG ASN C 359	9.815 56.559 104.061 1.00 57.06	C
		OD1 ASN C 359	9.530 56.230 105.237 1.00 61.37	0
		ND2 ASN C 359	10.443 57.691 103.772 1.00 57.61	N
		N TRP C 360	9.568 53.055 101.326 1.00 44.98	N C
		CA TRP C 360	8.980 51.992 100.530 1.00 43.27 9.436 50.637 101.030 1.00 43.73	C
		C TRP C 360 O TRP C 360		0
		CB TRP C 360	9.485 52.208 99.101 1.00 42.81	Č
		CG TRP C 360	9,293 50,969 98.261 1.00 43.02	Č
		CD1 TRP C 360	8.121 50.582 97.690 1.00 42.68	Č
		CD2 TRP C 360	10.270 49.978 97.909 1.00 42.05	С
		NE1 TRP C 360	8.335 49.411 97.017 1.00 43.15	N
		CE2 TRP C 360	9.632 49.020 97.128 1.00 42.10	С
		CE3 TRP C 360	11.619 49.812 98.190 1.00 42.67	С
ATOM	4215	CZ2 TRP C 360	10.261 47.902 96.606 1.00 42.59	C
ATOM	4216	CZ3 TRP C 360	12.278 48.711 97.685 1.00 43.71	С
		CH2 TRP C 360	11.598 47.767 96.899 1.00 43.79	C
		N ALA C 361	10.732 50.463 101.287 1.00 43.63	N
-		CA ALA C 361	11.262 49.197 101.739 1.00 44.41	C
		C ALA C 361	10.474 48.726 102.959 1.00 46.03	C
			10.110 47.541 103.017 1.00 45.76	. C
			12.745 49.292 102.036 1.00 43.71	. N
		N LYS C 362 CA LYS C 362	10.182 49.624 103.894 1.00 47.55 9.463 49.250 105.089 1.00 50.72	C
		C LYS C 362	8.117 48.616 104.849 1.00 51.32	c
		O LYS C 362	7.705 47.864 105.734 1.00 52.47	Ö
		CB LYS C 362	9.354 50.432 106.038 1.00 53.23	C
		CG LYS C 362	10.720 50.832 106.594 1.00 56.10	С
		CD LYS C 362	11.155 49.773 107.599 1.00 60.05	С
		CE LYS C 362	11.762 50.371 108.869 1.00 62.37	С
		NZ LYS C 362	11.973 49.344 109.950 1.00 63.33	N
		N ARG C 363	7.456 48.823 103.745 1.00 51.32	N
		CA ARG C 363	6.186 48.226 103.427 1.00 52.74	С
		C ARG C 363	6.288 47.007 102.539 1.00 51.87	C
		O ARG C 363	5.238 46.502 102.129 1.00 53.22	0
ATOM	4236	CB ARG C 363	5.351 49.253 102.657 1.00 56.62	С

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ATOM	1227	CG ARG C 363	6,006 50.631 102.784 1.00 62.69	С
		CD ARG C 363	5.368 51.299 104.018 1.00 68.16	Č
		NE ARG C 363	3,954 51.463 103.640 1.00 73.89	N
		CZ ARG C 363	3.622 52.373 102.697 1.00 77.79	Ċ
		NH1 ARG C 363	4.613 53.120 102.163 1.00 78.54	N
			2.326 52.501 102.337 1.00 78.75	N
		NH2 ARG C 363	7.443 46.512 102.137 1.00 50.42	N
ATOM		N VAL C 364	7.443 46.312 102.137 1.00 30.42	C
ATOM		CA VAL C 364	7.152 44.136 102.175 1.00 48.62	c
ATOM		C VAL C 364		Ö
		O VAL C 364	7.960 43.818 103.056 1.00 49.16	
ATOM		CB VAL C 364	8.758 45.196 100.552 1.00 47.54	C
ATOM		CG1 VAL C 364	8.932 43.867 99.857 1.00 46.99	C
		CG2 VAL C 364	8.826 46.340 99.567 1.00 47.58	C
		N PRO C 365	6.032 43.475 102.044 1.00 48.21	N
ATOM		CA PRO C 365	5.681 42.339 102.907 1.00 48.44	С
ATOM		C PRO C 365	6.876 41.471 103.242 1.00 48.67	С
ATOM		O PRO C 365	7.614 41.066 102.349 1.00 49.90	0
		CB PRO C 365	4.552 41.591 102.187 1.00 47.40	C
ATOM		CG PRO C 365	3.903 42.813 101.550 1.00 48.29	C
ATOM		CD PRO C 365	5.000 43.764 101.059 1.00 47.57	С
		N GLY C 366	7.125 41.223 104.524 1.00 48.37	N
ATOM		CA GLY C 366	8.198 40.394 105.005 1.00 47.61	С
ATOM	4259	C GLY C 366	9.486 41.099 105.359 1.00 47.49	С
ATOM		O GLY C 366	10.295 40.559 106.123 1.00 48.03	О
ATOM	4261	N PHE C 367	9.712 42.282 104.809 1.00 46.58	N
ATOM	4262	CA PHE C 367	10.945 43.027 105.006 1.00 45.91	С
ATOM	4263	C PHE C 367	11.205 43.352 106.462 1.00 46.07	С
<b>ATOM</b>		O PHE C 367	12.240 43.121 107.078 1.00 46.31	Ο
ATOM	4265	CB PHE C 367	10.898 44.331 104.205 1.00 45.19	С
ATOM	4266	CG PHE C 367	12.177 45.108 104.254 1.00 45.43	С
ATOM	4267	CD1 PHE C 367	13.256 44.686 103.505 1.00 44.99	С
ATOM	4268	CD2 PHE C 367	12.322 46.248 105.045 1.00 45.56	С
<b>ATOM</b>	4269	CE1 PHE C 367	14.457 45.378 103.529 1.00 44.64	С
<b>ATOM</b>	4270	<b>CE2 PHE C 367</b>	13.512 46.938 105.070 1.00 45.15	С
<b>ATOM</b>	4271	CZ PHE C 367	14.587 46.507 104.302 1.00 44.85	С
ATOM	4272	N VAL C 368	10.183 43.916 107.063 1.00 46.69	N
<b>ATOM</b>	4273	CA VAL C 368	10.167 44.342 108.456 1.00 48.15	С
<b>ATOM</b>	4274	C VAL C 368	10.370 43.209 109.433 1.00 49.45	С
ATOM	4275	O VAL C 368	10.729 43.461 110.576 1.00 51.13	Ο
<b>ATOM</b>	4276	CB VAL C 368	8.839 45.093 108.697 1.00 47.28	С
<b>ATOM</b>	4277	CG1 VAL C 368	8.130 44.630 109.922 1.00 46.30	С
ATOM	4278	CG2 VAL C 368	9.166 46.584 108.675 1.00 47.60	С
		N ASP C 369	10.179 41.953 109.060 1.00 49.63	N
		CA ASP C 369	10.429 40.828 109.904 1.00 49.20	С
ATOM		C ASP C 369	11.912 40.582 110.004 1.00 47.87	С

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ATOM	4282	O ASP C 369	12.265 39.674 110.747 1.00 50.06	0
ATOM		CB ASP C 369	9.807 39.560 109.326 1.00 52.94	С
ATOM		CG ASP C 369	8.306 39.646 109.140 1.00 57.07	С
ATOM		OD1 ASP C 369	7.536 40.253 109.942 1.00 58.15	0
ATOM		OD2 ASP C 369	7.883 39.050 108.107 1.00 59.37	0
ATOM		N LEUC 370	12.821 41.214 109.311 1.00 46.81	N
ATOM	_	CA LEUC 370	14.258 40.966 109.428 1.00 45.04	C
ATOM		C LEU C 370	14.866 41.839 110.513 1.00 43.57	С
ATOM		O LEUC 370	14.254 42.837 110.910 1.00 43.75	Ο
ATOM	4291		14.890 41.285 108.071 1.00 45.57	C
ATOM	4292	CG LEU C 370	14.408 40.389 106.933 1.00 45.97	C
ATOM	4293	CD1 LEU C 370	15.101 40.776 105.637 1.00 46.19	С
ATOM	4294	CD2 LEU C 370	14.724 38.931 107.276 1.00 45.91	С
<b>ATOM</b>	4295	N THR C 371	16.039 41.536 111.036 1.00 42.53	N
<b>ATOM</b>	4296	CA THR C 371	16.580 42.386 112.100 1.00 41.92	С
<b>ATOM</b>	4297	C THR C 371	16.872 43.746 111.509 1.00 42.67	С
ATOM	4298		17.204 43.891 110.332 1.00 43.23	0
ATOM		CB THR C 371	17.873 41.796 112.640 1.00 42.10	C
ATOM		OG1 THR C 371	18.638 41.467 111.456 1.00 43.55	0
ATOM		CG2 THR C 371	17.637 40.557 113.466 1.00 41.52	C
ATOM		N LEUC 372	16.806 44.784 112.334 1.00 43.35	N
ATOM		CA LEU C 372	17.071 46.123 111.810 1.00 43.84	C
ATOM		C LEUC 372	18.357 46.185 111.004 1.00 44.86	C
ATOM		O LEU C 372	18.366 46.867 109.970 1.00 44.98	O C
ATOM		CB LEU C 372	17.024 47.102 112.965 1.00 42.98	C.
ATOM		CG LEU C 372	15.695 47.307 113.677 1.00 41.37 15.874 48.209 114.886 1.00 41.90	C
ATOM		CD1 LEU C 372	14.703 47.968 112.755 1.00 40.39	C
ATOM		CD2 LEU C 372 N HIS C 373	19.435 45.513 111.409 1.00 45.75	N
ATOM		CA HIS C 373	20,661 45.607 110.630 1.00 47.06	Ċ
ATOM ATOM		C HIS C 373	20.502 44.905 109.308 1.00 46.38	Č
ATOM		O HIS C 373	21.005 45.465 108.331 1.00 45.68	Ö
		CB HIS C 373	21.832 45.143 111.475 1.00 50.24	C
		CG HIS C 373	22.249 46.192 112.465 1.00 52.68	·C
		ND1 HIS C 373	21.884 46.194 113.800 1.00 53.78	N
		CD2 HIS C 373	22.999 47.288 112.334 1.00 53.37	С
		CE1 HIS C 373	22.421 47.255 114.401 1.00 54.11	С
		NE2 HIS C 373	23.112 47.959 113.519 1.00 54.30	N
		N ASP C 374	19.792 43.778 109.258 1.00 45.87	N
		CA ASP C 374	19.599 43.113 107.963 1.00 45.03	С
		C ASP C 374	18.832 43.997 107.004 1.00 44.25	C
		O ASP C 374	19.180 44.045 105.812 1.00 44.05	Ο
		CB ASP C 374	18.986 41.731 108.142 1.00 46.40	С
ATOM	4325	CG ASP C 374	20.139 40.886 108.665 1.00 48.80	С
ATOM	4326	OD1 ASP C 374	21.283 41.356 108.487 1.00 49.03	Ο

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ATOM	4462 N LEU C 391	14.058 53.497 86.851 1.00 42.39	N
ATOM	4463 CA LEU C 391	14.309 54.343 85.679 1.00 42.48	С
ATOM	4464 C LEU C 391	13.889 53.586 84.434 1.00 43.75	С
ATOM	4465 O LEUC 391	13.060 54.004 83.635 1.00 44.31	О
		15.790 54.665 85.609 1.00 42.32	С
ATOM	4467 CG LEU C 391	16.325 55.261 84.318 1.00 42.43	С
ATOM	4468 CD1 LEU C 391	15.626 56.583 84.058 1.00 42.19	С
ATOM	4469 CD2 LEU C 391	17.840 55.475 84.358 1.00 42.78	С
ATOM	4470 N VAL C 392	14.451 52.387 84.261 1.00 44.61	N
ATOM	4471 CA VAL C 392	14.127 51.568 83.101 1.00 45.11	С
ATOM	4472 C VAL C 392	12.622 51.507 82.873 1.00 46.00	С
ATOM	4473 O VAL C 392	12.078 51.724 81.787 1.00 46.72	Ο
ATOM	4474 CB VAL C 392	14.752 50.167 83.237 1.00 43.59	С
ATOM	4475 CG1 VAL C 392	14.210 49.215 82.193 1.00 43.32	С
ATOM	4476 CG2 VAL C 392	16.262 50.250 82.999 1.00 42.75	С
ATOM	4477 N TRP C 393	11.902 51.174 83.924 1.00 46.93	N
ATOM	4478 CA TRP C 393	10.453 51.019 83.882 1.00 48.43	C
	4479 C TRP C 393		С
ATOM	4480 O TRP C 393	8.759 52.185 82.700 1.00 50.67	0
ATOM	4481 CB TRP C 393	9.937 50.621 85.262 1.00 48.30	С
ATOM	4482 CG TRP C 393	8.481 50.845 85.442 1.00 48.18	C
ATOM	4483 CD1 TRP C 393	7.912 51.799 86.217 1.00 49.07	С
ATOM	4484 CD2 TRP C 393	7.408 50.122 84.849 1.00 48.75	С
ATOM	4485 NE1 TRP C 393	6.537 51.695 86.155 1.00 49.00	N
ATOM	4486 CE2 TRP C 393	6.206 50.675 85.324 1.00 48.09	С
ATOM	4487 CE3 TRP C 393	7.349 49.030 83.968 1.00 49.78	С
ATOM	4488 CZ2 TRP C 393	4.957 50.202 84.956 1.00 48.08	С
ATOM	4489 CZ3 TRP C 393	6.099 48.547 83.591 1.00 49.68	С
ATOM	4490 CH2 TRP C 393	4.928 49.138 84.089 1.00 49.25	C
ATOM	4491 N ARG C 394	10.139 53.406 84.060 1.00 48.09	Ν
ATOM	4492 CA ARG C 394	9.450 54.634 83.700 1.00 47.92	C
ATOM	4493 C ARG C 394	9.934 55.088 82.344 1.00 49.43	С
ATOM	4494 O ARG C 394	9.287 55.925 81.730 1.00 51.46	O
ATOM	4495 CB ARG C 394	9.503 55.746 84.710 1.00 46.47	С
ATOM	4496 CG ARG C 394	10.763 56.081 85.415 1.00 45.70	С
ATOM	4497 CD ARG C 394	10.566 57.207 86.424 1.00 44.60	С
ATOM	4498 NE ARG C 394	11.920 57.710 86.742 1.00 44.81	N
ATOM	4499 CZ ARG C 394	12.693 57.162 87.681 1.00 43.57	С
ATOM	4500 NH1 ARG C 394	12.145 56.129 88.322 1.00 43.13	N
ATOM	4501 NH2 ARG C 394	13.896 57.673 87.883 1.00 41.36	N
ATOM	4502 N SER C 395	11.021 54.572 81.810 1.00 51.47	N
ATOM	4503 CA SER C 395	11.529 55.002 80.516 1.00 51.90	С
ATOM	4504 C SER C 395	10.991 54.173 79.388 1.00 53.62	С
	4505 O SER C 395	11.334 54.434 78.247 1.00 54.61	Ο
	4506 CB SER C 395	13.065 54.848 80.552 1.00 50.43	С

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A TON	4507 OC SER C 205	13.612 55.991 81.184 1.00 48.96	0
		10.218 53.150 79.665 1.00 56.89	
ATOM	4500 C1 MET C 396	9.697 52.238 78.670 1.00 60.23	C
ATOM	4510 C MET C 396	9.095 52.842 77.413 1.00 63.30	č
		9.523 52.504 76.297 1.00 63.66	
ATOM	4511 O WET C 396	8 583 51 406 79 298 1 00 59 55	C
ATOM	4512 CB NET C 396	8.583 51.406 79.298 1.00 59.55 8.723 49.930 79.002 1.00 59.80	Č
ATOM	4514 SD MET C 396	7.886 49.083 80.359 1.00 61.85	S
ATOM	4515 CE MET C 396	6.596 48.204 79.499 1.00 61.89	
ATOM	4516 N GLUC 397	8.110 53.729 77.604 1.00 66.03	N
ATOM	4517 CA GLU C 397	7.439 54.322 76.470 1.00 69.27	C
ATOM	4518 C GLU C 397	8.151 55.504 75.901 1.00 67.82	С
		7.474 56.429 75.435 1.00 69.29	
ATOM	4520 CB GLU C 397	6.018 54.786 76.785 1.00 74.53	С
ATOM	4521 CG GLU C 397	6.018 54.786 76.785 1.00 74.53 5.187 53.758 77.541 1.00 81.19	C
ATOM	4522 CD GLU C 397	5.613 53,797 79.002 1.00 85.34	С
		6.269 54.817 79.359 1.00 86.81	0
		5.316 52.820 79.737 1.00 88.67	
		9.452 55.666 75.936 1.00 65.73	N
		10.154 56.801 75.368 1.00 64.19	
		11.390 56.162 74.750 1.00 63.33	
ATOM	4528 O HIS C 398	12.489 56.333 75.265 1.00 64.80	0
ATOM	4529 CB HIS C 398	10.584 57.864 76.359 1.00 65.69	C
		9.454 58.536 77.071 1.00 67.75 8.465 57.788 77.699 1.00 68.11	
		9.121 59.824 77.286 1.00 68.37	
ATOM	4533 CF1 HIS C 398	7 559 58 547 78 254 1 00 68 33	Č
ATOM	4534 NE2 HIS C 398	7.559 58.547 78.254 1.00 68.33 7.943 59.791 78.021 1.00 69.24	N
ATOM	4535 N PRO C 399	11.169 55.409 73.695 1.00 61.57	N
		12.201 54.677 72.989 1.00 60.18	
		13.406 55.548 72.785 1.00 59.34	
	4538 O PRO C 399	13.227 56.719 72.471 1.00 60.76	0
<b>ATOM</b>	4539 CB PRO C 399	11.624 54.256 71.635 1.00 60.20	С
	4540 CG PRO C 399	10.177 54.105 72.045 1.00 61.13	С
	4541 CD PRO C 399	9.883 55.172 73.063 1.00 61.15	C
	4542 N GLY C 400	14.584 55.028 73.029 1.00 58.02	N
	4543 CA GLY C 400	15.779 55.810 72.817 1.00 57.60	C
	4544 C GLY C 400	16.055 56.848 73.866 1.00 57.41	C
	4545 O GLY C 400	17.142 57.465 73.774 1.00 59.48	0
	4546 N LYS C 401	15.168 57.029 74.824 1.00 55.91	N
	4547 CA LYS C 401 4548 C LYS C 401	15.375 58.004 75.873 1.00 56.17 15.214 57.440 77.288 1.00 54.71	C C
	4549 O LYS C 401	13.214 37.440 77.288 1.00 34.71 14.614 56.395 77.534 1.00 53.87	0
	4550 CB LYS C 401	14.325 59.092 75.773 1.00 58.67	C
	4551 CG LYS C 401		C
AIOM	4331 CO LIB C 401	13.203 32.073 (FF,F) 1.00 01.04	•

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ATOM	4642 CZ ARG C 412	25.373 55.780 72.193 1.00 67.73	C
ATOM	4643 NH1 ARG C 412	25.379 56.961 71.564 1.00 68.04	N
ATOM	4644 NH2 ARG C 412	26.531 55.145 72.370 1.00 67.64	N
ATOM	4645 N ASN C 413	22.590 60.264 73.461 1.00 67.18	N
ATOM	4646 CA ASN C 413	23.727 61.134 73.215 1.00 69.57	C
ATOM	4647 C ASN C 413	24.062 62.069 74.338 1.00 68.89	C 0
ATOM	4648 U ASN C 413	25.249 62.371 74.517 1.00 69.37	C
ATOM	4649 CB ASN C 413	23.457 61.894 71.902 1.00 73.23 23.211 60.796 70.856 1.00 76.66	C
ATOM	4651 OD1 ASN C 413	24.175 60.090 70.514 1.00 77.59	Ö
ATOM	4652 ND2 ASN C 413	21.937 60.700 70.451 1.00 78.09	N
ATOM	4653 N GLN C 414	23.126 62.512 75.161 1.00 67.79	N
ATOM	4654 CA GLN C 414	23.439 63.399 76.274 1.00 67.35	
ATOM	4655 C GLN C 414	24.282 62.671 77.308 1.00 67.26	С
ATOM	4656 O GLN C 414	24.986 63.252 78.133 1.00 66.80	0
ATOM	4657 CB GLN C 414	22.170 63.973 76.860 1.00 68.30	С
ATOM	4658 CG GLN C 414	21.127 64.314 75.798 1.00 69.45	С
		20.117 65.274 76.396 1.00 70.67	С
ATOM	4660 OE1 GLN C 414	18.908 65.040 76.412 1.00 71.62	0
ATOM	4661 NE2 GLN C 414	20.685 66.362 76.900 1.00 71.81	N
ATOM	4662 N GLY C 415	24.280 61.344 77.244 1.00 67.32	N
		25.114 60.498 78.069 1.00 67.57	C
ATOM	4664 C GLY C 415	26.543 60.925 77.798 1.00 67.85	C
		27.295 61.154 78.738 1.00 68.28	O N
ATOM	4666 N LYS C 416	26.974 61.147 76.566 1.00 69.42	C
	4668 C LYS C 416	28.343 61.564 76.260 1.00 70.20 28.826 62.756 77.069 1.00 68.84	c
ATOM	4660 O IVS C 416	30.035 62.973 77.197 1.00 68.46	Ö
ATOM	4670 CR I VS C 416	28.536 61.814 74.774 1.00 72.02	C
ATOM	4671 CG LYS C 416	27.801 60.834 73.887 1.00 75.13	Ċ
ATOM	4672 CD LYS C 416	28.735 60.255 72.828 1.00 78.53	С
	4673 CE LYS C 416	28.299 60.701 71.428 1.00 80.96	C
	4674 NZ LYS C 416	27.171 59.853 70.902 1.00 82.97	N
ATOM	4675 N CYS C 417	27.957 63.544 77.671 1.00 67.72	N
	4676 CA CYS C 417	28.400 64.669 78.473 1.00 68.04	С
	4677 C CYS C 417	29.289 64.173 79.591 1.00 65.78	C
	4678 O CYS C 417	30.319 64.804 79.839 1.00 66.63	0
	4679 CB CYS C 417	27.189 65.495 78.933 1.00 70.16	C
	4680 SG CYS C 417	26.344 66.190 77.467 1.00 75.80	S
	4681 N VAL C 418	28.954 63.094 80.279 1.00 63.41	N C
	4682 CA VAL C 418	29.782 62.604 81.370 1.00 61.12 30.653 61.452 80.918 1.00 60.84	C
	4683 C VAL C 418	30.146 60.621 80.184 1.00 60.27	0
	4684 O VAL C 418 4685 CB VAL C 418	28.910 62.163 82.549 1.00 60.20	C
	4686 CG1 VAL C 418	29.739 61.551 83.665 1.00 60.01	C
A I OIM	4000 CG1 VAL C 410	25.735 01.551 05.005 1.00 00.01	-

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ATOM	4687	CG2 VAL C 418	28.137 63.359 83.076 1.00 59.97	С
<b>ATOM</b>	4688	N GLU C 419	31.894 61.419 81.335 1.00 62.11	N
ATOM	4689	CA GLU C 419	32.844 60.376 81.019 1.00 64.89	С
ATOM	4690	C GLU C 419	32.362 58.995 81.400 1.00 64.14	С
ATOM	4691	O GLU C 419	31.817 58.720 82.462 1.00 64.65	Ο
ATOM	4692	CB GLU C 419	34.097 60.663 81.830 1.00 69.95	С
<b>ATOM</b>	4693	CG GLU C 419	35.415 60.468 81.108 1.00 77.04	С
ATOM	4694	CD GLU C 419	36.572 60.336 82.092 1.00 82.02	С
ATOM			36.507 60.945 83.209 1.00 84.55	0
ATOM	4696	OE2 GLU C 419	37.561 59.616 81.759 1.00 84.42	0
		N GLY C 420		N
		CA GLY C 420		С
		C GLY C 420		С
			30.235 55.276 81.342 1.00 64.98	0
			29.655 57.314 80.838 1.00 62.92	N
		CA MET C 421		С
ATOM		C MET C 421		С
ATOM	4704			0
ATOM			27.639 58.571 81.229 1.00 62.59	С
	4706	CG MET C 421	27.591 58.918 82.704 1.00 64.61	С
			25.913 58.610 83.314 1.00 67.20	S
			25.173 60.208 82.895 1.00 66.86	С
			27.896 56.713 78.674 1.00 59.89	N
			27.177 56.240 77.518 1.00 59.46	C.
		C VAL C 422		С
			25.812 54.359 77.160 1.00 58.65	0
			27.919 56.440 76.175 1.00 60.40	С
ATOM	4714	CG1 VAL C 422	26.932 56.991 75.156 1.00 61.42	С
ATOM	4715	CG2 VAL C 422	29.108 57.357 76.338 1.00 61.57	С
			27.910 53.993 78.049 1.00 58.67	N
			27.762 52.547 78.109 1.00 58.29	С
ATOM	4718	C GLU C 423	26.674 52.185 79.114 1.00 55.80	С
ATOM			25.911 51.254 78.862 1.00 56.05	0
		CB GLU C 423	29.023 51.835 78.541 1.00 62.43	С
		CG GLU C 423	30.178 52.163 77.618 1.00 69.18	С
		CD GLU C 423	30.915 53.376 78.163 1.00 72.99	С
ATOM	4723	OE1 GLU C 423	30.415 54.513 78.012 1.00 74.11	0
ATOM	4724	OE2 GLU C 423	32.004 53.165 78.762 1.00 76.42	0
ATOM	4725	N ILE C 424	26.662 52.944 80.214 1.00 51.13	N
ATOM	4726	<b>CA ILE C 424</b>	25.646 52.689 81.221 1.00 47.44	С
		C ILE C 424	24.324 53.032 80.585 1.00 47.25	С
		O ILE C 424	23.394 52.213 80.556 1.00 48.16	0
		CB ILE C 424	26.040 53.450 82.464 1.00 46.56	С
		CG1 ILE C 424	27.332 52.804 82.970 1.00 46.07	C
		CG2 ILE C 424	25.006 53.384 83.575 1.00 47.25	С

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ATOM	4732	CD1 ILE C 424	27.866 53.608 84.134 1.00 47.35	С
<b>ATOM</b>	4733	N PHE C 425	24.189 54.195 79.974 1.00 46.49	N
<b>ATOM</b>	4734	CA PHE C 425	22.962 54.562 79.295 1.00 46.97	С
<b>ATOM</b>	4735	C PHE C 425	22.565 53.492 78.288 1.00 48.46	С
ATOM	4736	O PHE C 425	21.393 53.143 78.086 1.00 49.04	0
ATOM	4737	CB PHE C 425	23.180 55.885 78.557 1.00 46.87	C
ATOM	4738	CG PHE C 425	22.888 57.092 79.393 1.00 48.05	С
<b>ATOM</b>	4739	CD1 PHE C 425	23.145 57.065 80.762 1.00 48.83	C
<b>ATOM</b>	4740	CD2 PHE C 425	22.367 58.239 78.833 1.00 47.47	С
<b>ATOM</b>	4741	CE1 PHE C 425	22.893 58.154 81.559 1.00 48.88	C
<b>ATOM</b>	4742	CE2 PHE C 425	22.117 59.331 79.629 1.00 48.48	C
ATOM	4743	CZ PHE C 425	22.367 59.296 80.987 1.00 49.12	С
<b>ATOM</b>	4744	N ASP C 426	23.558 52.958 77.570 1.00 49.47	N
ATOM	4745	CA ASP C 426	23.266 51.937 76.563 1.00 50.25	С
<b>ATOM</b>	4746	C ASP C 426	22.610 50.731 77.181 1.00 49.70	C
<b>ATOM</b>	4747	O ASP C 426	21.476 50.383 76.828 1.00 50.01	Ο
<b>ATOM</b>	4748	CB ASP C 426	24.551 51.740 75.805 1.00 52.75	С
<b>ATOM</b>	4749	CG ASP C 426	24.595 52.714 74.634 1.00 54.97	С
ATOM	4750	OD1 ASP C 426	23.525 53.281 74.348 1.00 55.90	Ο
ATOM	4751	OD2 ASP C 426	25.664 52.879 73.997 1.00 56.89	0
ATOM	4752	N MET C 427	23.221 50.136 78.189 1.00 48.67	N
<b>ATOM</b>	4753	CA MET C 427	22.654 49.011 78.926 1.00 46.57	С
<b>ATOM</b>	4754	C MET C 427	21.269 49.358 79.451 1.00 44.91	С
ATOM	4755	O MET C 427	20.324 48.563 79.360 1.00 43.81	Ο
			23.601 48.677 80.073 1.00 47.06	С
<b>ATOM</b>	4757	CG MET C 427	24.878 48.082 79.506 1.00 48.41	С
<b>ATOM</b>	4758	SD MET C 427	25.971 47.555 80.836 1.00 51.63	S
<b>ATOM</b>	4759	CE MET C 427	26.608 49.120 81.414 1.00 49.68	C
ATOM	4760	N LEU C 428	21.153 50.574 80.004 1.00 43.29	N
ATOM	4761	CA LEUC 428	19.838 50.987 80.499 1.00 42.10	С
ATOM	4762	C LEU C 428	18.822 50.985 79.362 1.00 42.51	C
ATOM			17.739 50.400 79.519 1.00 43.36	О
			19.930 52.326 81.199 1.00 40.36	С
		CG LEU C 428		С
		CD1 LEU C 428	20.986 53.753 82.919 1.00 40.04	С
		CD2 LEU C 428	19.870 51.656 83.622 1.00 39.72	С
		N LEU C 429	19.151 51.560 78.204 1.00 42.16	N
		CA LEUC 429	18.183 51.592 77.113 1.00 41.54	С
		C LEU C 429	17.793 50.203 76.669 1.00 42.36	С
ATOM		O LEU C 429	16.604 49.871 76.501 1.00 42.94	Ο
		CB LEU C 429	18.718 52.463 76.002 1.00 41.60	С
		CG LEU C 429	18.748 53.963 76.311 1.00 41.87	С
		CD1 LEU C 429	19.684 54.692 75.361 1.00 42.41	С
		CD2 LEU C 429	17.347 54.549 76.281 1.00 40.73	С
ATOM	4776	N ALA C 430	18.796 49.343 76.515 1.00 42.18	N

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ATOM	4777 CA ALA C 430	18.544 47.963 76.137 1.00 42.04	С
	4778 C ALA C 430	17.580 47.280 77.101 1.00 42.71	С
ATOM		16.751 46.465 76.666 1.00 44.50	0
ATOM	4780 CB ALA C 430	19.866 47.211 76.195 1.00 42.17	С
ATOM	4781 N THR C 431	17.670 47.540 78.401 1.00 41.61	N
ATOM	4782 CA THR C 431	16.764 46.859 79.309 1.00 41.93	С
ATOM		15.378 47.412 79.090 1.00 42.69	С
ATOM		14.347 46.744 79.063 1.00 41.58	0
	4785 CB THR C 431		C
	4786 OG1 THR C 431	18.546 46.950 80.878 1.00 44.44	0
ATOM		16.344 46.278 81.723 1.00 40.93	C
	4788 N SER C 432	15.404 48.745 78.942 1.00 45.20	N
	4789 CA SER C 432	14.149 49.490 78.767 1.00 46.82	C C
	4790 C SER C 432	13.390 48.962 77.561 1.00 46.53 12.191 48.710 77.540 1.00 46.14	0
ATOM		14.392 50.986 78.698 1.00 47.74	C
ATOM	4792 CB SER C 432 4793 OG SER C 432	13.074 51.509 78.440 1.00 50.00	0
	4794 N SER C 433	14.150 48.747 76.514 1.00 47.34	N
ATOM		13.668 48.149 75.292 1.00 49.60	Ĉ
ATOM		13.123 46.748 75.472 1.00 49.87	Č
	4797 O SER C 433		Ö
		14.950 48.089 74.459 1.00 51.76	С
	4799 OG SER C 433	14.471 47.977 73.129 1.00 57.08	Ο
ATOM		13.863 45.867 76.147 1.00 51.89	N
ATOM		13.411 44.512 76.446 1.00 53.04	С
<b>ATOM</b>	4802 C ARG C 434	12.110 44.574 77.248 1.00 53.63	С
<b>ATOM</b>	4803 O ARG C 434	11.188 43.778 77.007 1.00 52.87	O
	4804 CB ARG C 434	14.457 43.666 77.163 1.00 53.71	C
		13.927 42.293 77.511 1.00 56.12	C
		14.802 41.123 77.122 1.00 58.81	C
ATOM	4807 NE ARG C 434	14.084 39.828 77.305 1.00 60.35	N
	4808 CZ ARG C 434	13.212 39.481 76.350 1.00 61.02	C N
	4809 NH1 ARG C 434		N
	4810 NH2 ARG C 434	11.994 45.517 78.200 1.00 54.32	N
	4811 N PHE C 435 4812 CA PHE C 435	10.747 45.613 78.954 1.00 55.85	C
_	4813 C PHE C 435	9.604 45.980 78.009 1.00 57.99	c
	4814 O PHE C 435	8.488 45.463 78.148 1.00 57.42	Ö
	4815 CB PHE C 435	10.833 46.587 80.108 1.00 55.50	C
	4816 CG PHE C 435	11.450 46.066 81.373 1.00 55.59	Č
	4817 CD1 PHE C 435	11.748 44.719 81.548 1.00 55.40	C
	4818 CD2 PHE C 435	11.735 46.941 82.410 1.00 54.85	С
	4819 CE1 PHE C 435	12.330 44.252 82.692 1.00 54.88	С
	4820 CE2 PHE C 435	12.312 46.512 83.573 1.00 54.54	С
	4821 CZ PHE C 435	12.609 45.163 83.698 1.00 55.69	С

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ATOM	4822	N ARG C 436	9.895 46.864 77.039 1.00 60.12	N
			8.905 47.250 76.049 1.00 62.03	С
<b>ATOM</b>	4824	C ARG C 436	8.479 46.028 75.247 1.00 63.18	С
ATOM	4825	O ARG C 436	7.300 45.695 75.167 1.00 63.07	Ο
<b>ATOM</b>	4826	CB ARG C 436	9.489 48.295 75.126 1.00 63.26	С
<b>ATOM</b>	4827	CG ARG C 436	8.479 49.271 74.577 1.00 65.79	С
<b>ATOM</b>	4828	CD ARG C 436	9.088 50.278 73.624 1.00 68.16	С
<b>ATOM</b>	4829	NE ARG C 436	10.145 51.074 74.245 1.00 69.88	N
ATOM	4830	CZ ARG C 436	11.413 51.012 73.842 1.00 71.48	С
ATOM	4831	NH1 ARG C 436	11.753 50.206 72.835 1.00 71.96	N
ATOM	4832	NH2 ARG C 436	12.343 51.753 74.446 1.00 72.39	N
ATOM	4833	N MET C 437	9.441 45.309 74.683 1.00 65.08	N
<b>ATOM</b>	4834	CA MET C 437	9.124 44.123 73.919 1.00 67.98	С
<b>ATOM</b>	4835	C MET C 437	8.298 43.091 74.651 1.00 66.52	С
ATOM	4836	O MET C 437	7.413 42.492 74.051 1.00 67.09	0
ATOM	4837	CB MET C 437	10.394 43.416 73.489 1.00 73.78	С
ATOM	4838	CG MET C 437	11.173 44.154 72.409 1.00 80.32	С
			12.348 43.010 71.647 1.00 87.14	S
ATOM	4840	CE MET C 437	13.497 42.566 72.961 1.00 84.82	С
ATOM	4841	N MET C 438	8.543 42.820 75.917 1.00 65.34	N
ATOM	4842	CA MET C 438	7.802 41.840 76.696 1.00 63.76	С
<b>ATOM</b>	4843	C MET C 438	6.488 42.370 77.246 1.00 62.74	С
ATOM	4844	O MET C 438	5.750 41.629 77.857 1.00 61.15	Ο
ATOM	4845	CB MET C 438	8.596 41.518 77.955 1.00 63.80	C
ATOM		CG MET C 438	9.993 41.010 77.625 1.00 63.23	С
			10.545 40.126 79.062 1.00 64.41	S
ATOM		CE MET C 438	9.130 39.254 79.688 1.00 64.16	С
ATOM		N ASN C 439	6.313 43.666 77.043 1.00 63.40	N
ATOM		CA ASN C 439	5.120 44.358 77.478 1.00 64.21	С
ATOM	4851	C ASN C 439		C
	4852			0
		CB ASN C 439	3.968 43.923 76.576 1.00 69.26	C
ATOM	4854	CG ASN C 439	2.734 44.729 76.957 1.00 74.42	C
			1.595 44.254 76.772 1.00 77.74	0
		ND2 ASN C 439	2.935 45.937 77.509 1.00 75.66	N
		N LEUC 440	5.842 44.507 79.721 1.00 59.76	N
		CA LEU C 440	5.897 44.300 81.147 1.00 58.34	С
		C LEUC 440	4.799 45.104 81.805 1.00 59.09	C
		O LEUC 440	4.699 46.294 81.566 1.00 58.96	0
		CB LEU C 440	7.262 44.697 81.689 1.00 57.06	C
		CG LEU C 440	7.481 44.715 83.192 1.00 55.81	C
		CD1 LEU C 440	7.505 43.319 83.760 1.00 55.18	C
		CD2 LEU C 440	8.759 45.460 83.518 1.00 55.68	C
		N GLN C 441	4.024 44.404 82.620 1.00 59.85	N
ATOM	4866	CA GLN C 441	2.934 45.032 83.333 1.00 60.62	С

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ATOM	4867	C GLN C 441	3.379 45.686 84.617 1.00 60.00	С
ATOM	4868	O GLN C 441	4.368 45.251 85.170 1.00 61.05	Ο
ATOM	4869	CB GLN C 441	1.983 43.920 83.748 1.00 63.02	С
<b>ATOM</b>	4870	CG GLN C 441	1.311 43.221 82.594 1.00 66.39	С
			0.784 44.199 81.570 1.00 68.71	С
<b>ATOM</b>	4872	OE1 GLN C 441	-0.225 44.840 81.864 1.00 71.08	0
<b>ATOM</b>	4873	NE2 GLN C 441	1.447 44.310 80.426 1.00 69.56	N
<b>ATOM</b>	4874	N GLY C 442	2.623 46.631 85.141 1.00 60.01	N
ATOM	4875	CA GLY C 442	2.979 47.285 86.401 1.00 57.82	С
<b>ATOM</b>	4876	C GLY C 442	2.938 46.301 87.546 1.00 56.23	С
			3.773 46.384 88.432 1.00 55.56	0
<b>ATOM</b>	4878	N GLU C 443	2.024 45.342 87.572 1.00 56.45	N
<b>ATOM</b>	4879	CA GLU C 443	1.958 44.388 88.679 1.00 57.44	С
<b>ATOM</b>	4880	C GLU C 443	3.253 43.564 88.662 1.00 55.03	С
ATOM	4881	O GLU C 443	3.793 43.215 89.709 1.00 54.58	0
<b>ATOM</b>	4882	CB GLU C 443	0.788 43.422 88.734 1.00 60.73	С
<b>ATOM</b>	4883	CG GLU C 443	-0.627 43.920 88.621 1.00 65.19	С
ATOM	4884	CD GLU C 443	-0.852 44.790 87.392 1.00 68.64	С
ATOM	4885	OE1 GLU C 443	-0.429 44.448 86.260 1.00 69.36	Ο
<b>ATOM</b>	4886	OE2 GLU C 443	-1.459 45.870 87.601 1.00 71.25	0
			3.711 43.263 87.453 1.00 52.22	N
<b>ATOM</b>	4388	CA GLU C 444	4.956 42.532 87.278 1.00 49.44	С
<b>ATOM</b>	4889	C GLU C 444	6.125 43.367 87.782 1.00 47.52	С
<b>ATOM</b>	4890	O GLU C 444	6.931 42.906 88.592 1.00 47.70	O
			5.146 42.200 85.811 1.00 48.97	С
ATOM	4892	CG GLU C 444	4.202 41.069 85.406 1.00 48.66	С
ATOM	4893	CD GLU C 444	4.329 40.783 83.920 1.00 48.63	С
			4.480, 41.780 83.171 1.00 47.53	Ο
			4.272 39.573 83.603 1.00 48.73	0
			6.177 44.609 87.346 1.00 45.52	N
			7.214 45.539 87.740 1.00 44.59	С
			7.390 45.590 89.250 1.00 45.53	С
			8.467 45.443 89.845 1.00 47.20	О
			6.914 46.942 87.235 1.00 42.98	С
		CG PHE C 445	7.774 48.008 87.831 1.00 42.70	C ·
			9.140 47.987 87.636 1.00 43.19	С
		CD2 PHE C 445		С
		CE1 PHE C 445		С
		CE2 PHE C 445	8.046 50.013 89.135 1.00 43.47	С
		CZ PHE C 445	9.412 49.976 88.910 1.00 44.42	С
		N VAL C 446		N
		CA VAL C 446	6.272 45.935 91.405 1.00 45.30	С
		C VAL C 446		С
			7.433 44.710 93.103 1.00 47.48	Ο
ATOM	4911	CB VAL C 446	4.837 46.404 91.699 1.00 44.57	С

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ATOM	4912	CG1 VAL C 446	4.019 45.522 92.584 1.00 43.76	С
ATOM	4913	CG2 VAL C 446	4.889 47.842 92.195 1.00 44.33	С
ATOM	4914	N CYS C 447	6.551 43.489 91.465 1.00 47.28	N
ATOM	4915	CA CYS C 447	7.038 42.253 92.052 1.00 48.53	С
ATOM	4916	C CYS C 447	8.544 42.111 91.882 1.00 49.06	С
ATOM			9.269 41.719 92.803 1.00 50.00	О
ATOM			6.383 41.069 91.346 1.00 50.22	С
ATOM		SG CYS C 447		S
ATOM		N LEU C 448		N
			10.478 42.283 90.394 1.00 45.53	С
ATOM	4922	C LEU C 448	11.266 43.194 91.312 1.00 44.33	С
ATOM			12.270 42.813 91.897 1.00 44.64	0
ATOM			10.747 42.680 88.961 1.00 45.46	С
ATOM	4925	CG LEU C 448	10.340 41.710 87.874 1.00 46.19	С
			10.637 42.390 86.536 1.00 47.62	C
ATOM	4927	CD2 LEU C 448	11.073 40.383 88.007 1.00 46.34	C
			10.776 44.420 91.456 1.00 42.83	Ν
ATOM	4929	CA LYS C 449	11.442 45.371 92.343 1.00 42.54	C
ATOM	4930	C LYS C 449	11.569 44.810 93.740 1.00 42.45	С
			12.616 44.935 94.366 1.00 42.82	Ο
<b>ATOM</b>		CB LYS C 449		С
ATOM			11.518 47.902 92.420 1.00 44.96	С
			10.682 48.858 93.233 1.00 45.78	С
ATOM	4935	CE LYS C 449	9.829 49.773 92.376 1.00 45.95	С
		NZ LYS C 449		N
			10.585 44.140 94.330 1.00 42.30	N
ATOM	4938	CA SER C 450	10.713 43.531 95.642 1.00 41.90	С
ATOM	4939		11.654 42.334 95.600 1.00 40.58	C
ATOM	4940		12.397 42.164 96.538 1.00 41.12	0
ATOM			9.389 42.962 96.170 1.00 43.19	C
ATOM			8.496 44.055 96.086 1.00 46.06	0
ATOM	4943	N ILEC 451	11.621 41.525 94.557 1.00 39.35	N·
ATOM			12.542 40.416 94.435 1.00 38.13	С
		C ILE C 451		C
		O ILE C 451	14.748 40.431 95.269 1.00 37.68	0
		CB ILE C 451	12.351 39.683 93.100 1.00 38.57	C
		CG1 ILE C 451	10.934 39.103 93.141 1.00 38.70	C
		CG2 ILE C 451	13.459 38.678 92.856 1.00 36.53	C
		CD1 ILE C 451	10.708 38.069 92.060 1.00 40.52	C
		N ILE C 452	14.213 42.084 93.786 1.00 36.55	N
		CA ILE C 452	15.543 42.703 93.834 1.00 36.20	C
		C ILE C 452	15.917 43.115 95.248 1.00 37.08	C
ATOM		4	16.998 42.826 95.733 1.00 37.44	0
		CB ILE C 452	15.659 43.928 92.914 1.00 34.94	C
ATOM	4956	CG1 ILE C 452	15.467 43.485 91.464 1.00 35.56	С

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			16.968 44.655 93.112 1.00 34.17	С
			15.721 44.467 90.341 1.00 34.41	С
		N LEU C 453		N
		CA LEU C 453	15.309 44.201 97.328 1.00 38.20	С
		C LEU C 453		C
		D LEU C 453		0
		CB LEU C 453		C
		CG LEU C 453	14.236 45.195 99.466 1.00 35.32 15.403 46.124 99.738 1.00 33.69	C C
			12.959 45.756 100.051 1.00 34.14	C
		N LEU C 454		N
		CA LEU C 454	15.147 40.758 98.959 1.00 43.72	Ċ
		LEU C 454		c
		LEU C 454	•	O
ATOM	4971 C	CB LEU C 454	13.853 39.905 99.059 1.00 43.87	С
ATOM	4972 C	G LEU C 454	12.778 40.568 99.923 1.00 44.26	С
			11.412 40.002 99.623 1.00 44.28	С
			13.149 40.345 101.376 1.00 44.75	С
		I ASN C 455		N
		CA ASN C 455	17.450 38.623 96.855 1.00 45.74	С
		ASN C 455		C O
		ASN C 455	19.726 38.337 96.800 1.00 50.93 17.014 37.961 95.565 1.00 44.52	C
		G ASN C 455		C
			18.469 37.593 93.781 1.00 45.37	o
			18,250 35,885 95,291 1,00 42,07	N
ATOM	4983 N	SER C 456	19.064 40.403 96.473 1.00 51.80	N
			20.440 40.851 96.248 1.00 54.85	С
		SER C 456		С
		SER C 456		0
			20.435 42.295 95.736 1.00 54.12	C
		G SER C 456 GLY C 457	20.138 42.329 94.360 1.00 52.76	O
		A GLY C 457	21.046 41.060 98.609 1.00 60.33 21.983 40.904 99.716 1.00 63.48	N C
		GLY C 457	21.824 39.630 100.506 1.00 65.50	C -
		GLY C 457	22.471 39.536 101.553 1.00 65.18	ŏ
		VAL C 458	21.007 38.692 100.047 1.00 68.21	N
		A VAL C 458	20.775 37.473 100.799 1.00 71.05	C
ATOM	4995 C	VAL C 458	21.980 36.607 101.035 1.00 75.07	С
ATOM	4996 O	VAL C 458	22.054 36.091 102.167 1.00 76.32	0
		B VAL C 458	19.575 36.686 100.270 1.00 69.84	С
		G1 VAL C 458	19.811 35.979 98.973 1.00 68.69	С
		G2 VAL C 458	19.138 35.706 101.359 1.00 69.73	C
		TYR C 459	22.958 36.441 100.166 1.00 79.58	N
AIOM	2001 C	A TYR C 459	24.146 35.635 100.364 1.00 83.85	С

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ATOM	5002 C TYR C 459	25.224 36.366 101.129 1.00 86.14	С
ATOM	5003 O TYR C 459	26.383 35.952 101.068 1.00 87.66	Ο
ATOM	5004 CB TYR C 459	24.818 35.195 99.022 1.00 85.85	С
ATOM	5005 CG TYR C 459	23.736 34.491 98.235 1.00 88.50	С
ATOM	5006 CD1 TYR C 459	22.830 35.301 97.561 1.00 89.49	С
ATOM	5007 CD2 TYR C 459	23.534 33.123 98.179 1.00 89.54	С
ATOM	5008 CE1 TYR C 459	21.809 34.664 96.927 1.00 90.75	С
ATOM	5009 CE2 TYR C 459	22.477 32.559 97.471 1.00 90.82	С
<b>ATOM</b>	5010 CZ TYR C 459	21.582 33.346 96.790 1.00 91.29	C
<b>ATOM</b>	5011 OH TYR C 459	20.497 32.907 96.064 1.00 91.89	0
	5012 N THR C 460		N
<b>ATOM</b>	5013 CA THR C 460	25.894 38.231 102.538 1.00 91.09	С
ATOM	5014 C THR C 460	25.316 38.723 103.849 1.00 92.44	C
ATOM			Ο
		26.361 39.420 101.681 1.00 91.40	С
		25.703 39.507 100.413 1.00 91.84	О
	5018 CG2 THR C 460		С
	5019 N PHE C 461		N
		24.018 38.287 105.816 1.00 95.54	С
	5021 C PHE C 461		C
ATOM		24.579 39.656 107.697 1.00 97.39	Ο
ATOM		22.859 37.323 106.179 1.00 95.11	C
ATOM		21.571 38.019 105.769 1.00 94.25	C
ATOM		21.517 39.404 105.732 1.00 93.75	С
ATOM	5026 CD2 PHE C 461	20.450 37.306 105.421 1.00 94.01	C
ATOM		20.379 40.066 105.358 1.00 93.81	С
ATOM		19.305 37.974 105.053 1.00 93.96	C
		19.254 39.353 105.016 1.00 93.71	С
	5030 N THR C 465		N
		24.660 32.726 112.031 1.00128.12	C
ATOM	5032 C THR C 465		C
ATOM	5033 O THR C 465		0
		25.798 31.732 112.320 1.00128.79	C
	5035 OG1 THR C 465	25.434 30.413 111.883 1.00129.06	0
	5036 CG2 THR C 465	26.164 31.714 113.795 1.00129.25	C
	5037 N LEU C 466	22.990 31.349 113.227 1.00125.02	N
	5038 CA LEU C 466	21.700 30.665 113.350 1.00122.24	C
	5039 C LEU C 466	20.539 31.629 113.107 1.00120.10	C
	5040 O LEUC 466	19.510 31.214 112.557 1.00120.29	0
ATOM		21.572 29.987 114.713 1.00122.49	C
	5045 N LYS C 467	20.684 32.909 113.481 1.00116.70	N
	5046 CA LYS C 467	19.670 33.922 113.224 1.00112.91	C
	5047 C LYS C 467	19.721 34.200 111.720 1.00108.82	С
ATOM		18.695 34.460 111.109 1.00108.56	0
ATOM	5049 CB LYS C 467	19.858 35.224 113.989 1.00114.52	С

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		18.591 36.061 114.190 1.00115.87	
		18.944 37.459 114.677 1.00117.42	
ATOM	5052 UE LYS C 467	18.789 37.702 116.175 1.00118.05 19.336 39.016 116.623 1.00117.84	C
ATOM	5054 N SER C 468	20.905 34.112 111.126 1.00103.95	N N
		21.085 34.318 109.705 1.00 99.66	
	5056 C SER C 468		•
		19.823 33.423 107.862 1.00 95.24	Ö
		22.564 34.322 109.314 1.00100.26	С
		23.212 35.441 109.875 1.00101.24	0
ATOM	5060 N LEUC 469	20.559 31.991 109.430 1.00 92.38	N
		19.967 30.829 108.764 1.00 89.30	С
	5062 C LEU C 469		C
		17.766 30.720 107.816 1.00 86.34	
		20.473 29.539 109.400 1.00 89.33	
		17.928 31.563 109.850 1.00 84.83	N C
		16.495 31.823 109.972 1.00 83.61 16.134 33.035 109.132 1.00 79.55	· ·
		15.088 33.047 108.489 1.00 78.82	
ATOM	5072 CB GLU C 470	16 139 31 901 111 440 1 00 87 71	C
ATOM	5073 CG GLU C 470	15.292 33.077 111.873 1.00 93.24	C
<b>ATOM</b>	5074 CD GLU C 470	15.355 33.290 113.380 1.00 96.76	С
		16.284 32.733 114.028 1.00 98.22	
		14.467 34.022 113.897 1.00 98.81	
		16.978 34.054 109.076 1.00 75.35	
		16.770 35.226 108.239 1.00 71.42	C
		16.811 34.789 106.767 1.00 70.18	
ATOM	5081 CR GLUC 4/1	16.028 35.203 105.917 1.00 70.00 17.840 36.278 108.472 1.00 70.12	O C
ATOM	5082 CG GLUC 471	17.934 36.974 109.788 1.00 68.28	C
		17.259 38.305 109.857 1.00 68.11	Č
	- · · · · · · · ·	17.694 39.296 109.273 1.00 67.82	O
		16.213 38.451 110.514 1.00 69.38	Ο
ATOM	5086 N LYS C 472	17.741 33.908 106.395 1.00 68.96	N
		17.819 33.410 105.031 1.00 67.47	C
	5088 C LYS C 472		C
	5089 O LYS C 472	16.002 32.905 103.630 1.00 64.82	0
	5090 CB LYS C 472	19.051 32.561 104.737 1.00 68.76	C
		20.339 33.368 104.695 1.00 70.99 21.463 32.567 104.073 1.00 73.75	C C
		22.800 32.870 104.073 1.00 73.73	C
		23.538 34.011 104.094 1.00 78.24	N
	5095 N ASP C 473		N
		14.833 31.037 105.206 1.00 64.30	C
		13.659 31.962 104.961 1.00 61.70	С
ATOM	5097 C ASP C 473	13.659 31.962 104.961 1.00 61.70	C

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ATON	M 5143	CA VAL C 478	8.785 35.397 100.877 1.00 50.99	С
ATON	<b>1</b> 5144	C VAL C 478	9.051 35.410 99.387 1.00 49.83	C
ATON	M 5145	O VAL C 478	8.164 35.608 98.569 1.00 49.34	Ο
ATON	<b>M</b> 5146	CB VAL C 478	9.272 36.682 101.553 1.00 51.01	С
ATON	M 5147	CG1 VAL C 478	8.626 37.917 100.977 1.00 51.00	С
ATON	<b>M</b> 5148	CG2 VAL C 478	8.998 36.543 103.040 1.00 50.78	С
ATON	<b>M</b> 5149	N LEU C 479	10.293 35.118 98.989 1.00 49.33	N
ATON	и 5150	CA LEUC 479	10.667 35.040 97.577 1.00 48.40	С
ATON	M 5151	C LEU C 479	9.793 34.022 96.824 1.00 49.73	С
ATON	M 5152	O LEU C 479	9.423 34.242 95.655 1.00 49.19	0
ATON	M 5153	CB LEU C 479	12.142 34.732 97.409 1.00 44.59	С
ATON	M 5154	CG LEU C 479	13.058 35.946 97.486 1.00 42.74	С
ATON	M 5155	CD1 LEU C 479	14.506 35.505 97.582 1.00 42.36	С
ATON	M 5156	CD2 LEU C 479	12.832 36.885 96.327 1.00 41.90	С
ATON	M 5157	N ASP C 480	9.427 32.915 97.493 1.00 50.12	N
ATON	M 5158	CA ASP C 480	8.558 31.937 96.863 1.00 50.18	С
ATON	A 5159	C ASP C 480	7.175 32.546 96.740 1.00 51.14	С
ATON	<b>A</b> 5160	O ASP C 480	6.523 32.390 95.717 1.00 51.29	0
ATON	M 5161	CB ASP C 480	8.488 30.649 97.631 1.00 50.11	С
ATON	И 5162	CG ASP C 480	9.741 29.825 97.574 1.00 51.36	С
ATON	<b>A</b> 5163	OD1 ASP C 480	10.591 29.903 96.676 1.00 52.08	0
ATON	<b>A</b> 5164	OD2 ASP C 480	9.927 29.000 98.488 1.00 52.79	0
ATON	<b>A</b> 5165	N LYS C 481	6.743 33.265 97.776 1.00 53.56	N
ATON	<b>A</b> 5166	CA LYS C 481	5.417 33.889 97.776 1.00 54.84	C
ATON	<b>1</b> 5167	C LYS C 481	5.340 34.861 96.607 1.00 53.95	С
ATON	A 5168	O LYS C 481	4.398 34.790 95.807 1.00 53.74	0
ATON	И 5169	CB LYS C 481	5.094 34.576 99.094 1.00 57.80	С
ATON	A 5170	CG LYS C 481	3.623 34.949 99.230 1.00 63.05	С
		CD LYS C 481	2.826 33.854 99.962 1.00 66.61	С
		CE LYS C 481	1.357 33.824 99.573 1.00 68.92	С
		NZ LYS C 481	1.120 34.517 98.248 1.00 71.39	N
		N ILE C 482		N
			6.371 36.660 95.352 1.00 49.12	С
		C ILE C 482		С
		O ILE C 482	5.783 36.297 93.085 1.00 47.95	0
		CB ILE C 482	7.460 37.713 95.455 1.00 48.89	С
		CG1 ILE C 482	7.192 38.602 96.668 1.00 49.17	С
		CG2 ILE C 482	7.483 38.626 94.244 1.00 49.02	С
		CD1 ILE C 482	8.459 38.975 97.400 1.00 50.45	С
		N THR C 483	7.081 34.753 93.952 1.00 47.76	N
		CA THR C 483		С
		C THR C 483	5.643 33.514 92.425 1.00 49.14	С
		O THR C 483	5.186 33.642 91.291 1.00 49.74	Ο
		CB THR C 483		С
ATON	И 5187	OG1 THR C 483	9.270 33.189 92.970 1.00 49.16	0

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5188	CG2 THR C 483	7.772 31.830 91.625 1.00 47.31	С
5189	N ASP C 484		N
			С
			С
5192	O ASP C 484	1.876 33.608 91.893 1.00 48.21	0
5193	CB ASP C 484	2.985 31.988 94.520 1.00 49.64	С
5194	CG ASP C 484	3.626 30.688 94.932 1.00 51.32	С
5195	OD1 ASP C 484	4.320 30.043 94.113 1.00 51.62	<b>O</b>
5196	OD2 ASP C 484	3.421 30.296 96.107 1.00 52.63	0
5197	N THR C 485	2.869 34.912 93.360 1.00 48.09	N
5198	CA THR C 485	2.119 36.086 92.938 1.00 47.03	С
5199	C THR C 485	2.339 36.321 91.465 1.00 47.25	С
5200	O THR C 485	1.385 36.554 90.749 1.00 47.41	0
5201	CB THR C 485	2.596 37.283 93.776 1.00 46.36	· C
			0
5203	CG2 THR C 485	1.807 38.518 93.441 1.00 45.66	С
			N
			С
			C
			0
			C
5209	CG LEU C 486		С
			C
5211	CD2 LEU C 486		С
			N
			С
			C
			0
			C
			C
			C
			C
			N
			C
			C
			0
			C
			C
			N
			C
			C
			N
			N
			C
5232	C LEU C 489	-0.908 36.854 86.262 1.00 58.89	С
	5189 5190 5191 5192 5193 5194 5195 5196 5197 5198 5199 5200 5201 5202 5203 5204 5205 5206 5207 5208 5209 5210 5211 5212 5213 5214 5215 5216 5217 5218 5219 5220 5221 5222 5223 5224 5225 5226 5227 5228 5229 5220 5221 5222 5223 5224 5225 5226 5227 5228 5229 5220 5221 5222 5223 5224 5225 5226 5227 5228 5229 5220 5221 5222 5223 5224 5225 5226 5227 5228 5229 5220 5221 5222 5223 5224 5225 5226 5227 5228 5229 5220 5221 5222 5223 5224 5225 5226 5227 5228 5229 5220 5221 5222 5223 5224 5225 5226 5227 5228 5229 5220 5221 5222 5223 5224 5225 5226 5227 5228 5229 5220 5221 5222 5223 5224 5225 5226 5227 5228 5229 5220 5221 5222 5223 5224 5225 5226 5227 5228 5229 5220 5220 5221 5222 5223 5224 5225 5226 5227 5228 5229 5229 5220 5220 5221 5222 5223 5224 5225 5226 5227 5228 5229 5229 5220 5220 5220 5220 5220 5220	5189 N ASP C 484 5190 CA ASP C 484 5191 C ASP C 484 5192 O ASP C 484 5193 CB ASP C 484 5194 CG ASP C 484 5195 OD1 ASP C 484 5196 OD2 ASP C 484 5197 N THR C 485 5198 CA THR C 485 5199 C THR C 485 5200 O THR C 485 5201 CB THR C 485 5201 CB THR C 485 5202 OG1 THR C 485 5203 CG2 THR C 485 5204 N LEU C 486 5205 CA LEU C 486 5206 C LEU C 486 5207 O LEU C 486 5208 CB LEU C 486 5209 CG LEU C 486 5210 CD1 LEU C 486 5210 CD1 LEU C 486 5211 CD2 LEU C 486 5212 N ILE C 487 5213 CA ILE C 487 5214 C ILE C 487 5215 O ILE C 487 5216 CB ILE C 487 5217 CG1 ILE C 487 5218 CG2 ILE C 487 5219 CD1 ILE C 487	7.772 31.830 91.625 1.00 47.31 4.946 32.989 93.446 1.00 49.27 3.557 32.562 93.251 1.00 48.63 2.691 33.722 92.790 1.00 48.18 1.876 33.608 91.893 1.00 48.21 2.985 31.988 94.520 1.00 49.64 3.626 30.688 94.932 1.00 51.32 4.320 30.043 94.113 1.00 51.62 3.626 30.688 94.932 1.00 51.32 4.320 30.043 94.113 1.00 51.62 3.626 30.688 94.932 1.00 51.32 4.320 30.043 94.113 1.00 51.62 3.421 30.296 96.107 1.00 52.63 2.869 34.912 93.360 1.00 48.09 2.119 36.086 92.938 1.00 47.03 2.869 34.912 93.360 1.00 48.09 2.119 36.086 92.938 1.00 47.03 2.869 34.912 93.360 1.00 48.09 2.119 36.086 92.938 1.00 47.03 2.869 34.912 93.360 1.00 48.09 2.119 36.086 92.938 1.00 47.03 2.869 34.912 93.360 1.00 46.06 2.473 36.870 95.137 1.00 46.36 2.473 36.870 95.137 1.00 46.36 2.473 36.870 95.137 1.00 45.66 3.584 36.243 91.012 1.00 49.46 3.584 36.243 91.012 1.00 49.46 3.584 36.243 91.012 1.00 49.46 3.143 35.935 87.777 1.00 55.65 321 32.66 34.223 88.942 1.00 52.22 2.545 33.226 88.170 1.00 53.78 1.00 43.24 31.33 33.494 88.230 1.00 54.55 4.043 33.494 88.230 1.00 55.65 3220 N HIS C 488 5222 C HIS C 488 5223 O N LEU C 489 5231 CA LEU C 489 5231

		ε <b>20</b> / <b>3</b> · ·	
ATOM	5233 O LEUC 489	-1.829 37.140 85.507 1.00 59.10	Ο
<b>ATOM</b>	5234 CB LEU C 489	0.330 38.360 87.856 1.00 57.52	С
	5235 CG LEU C 489		С
		1.542 40.042 89.206 1.00 58.98	С
<b>ATOM</b>	5237 CD2 LEU C 489	-0.894 40.271 88.863 1.00 57.71	С
<b>ATOM</b>	5238 N MET C 490	0.073 36.111 85.788 1.00 59.42	N
<b>ATOM</b>	5239 CA MET C 490	0.185 35.601 84.450 1.00 60.66	С
<b>ATOM</b>	5240 C MET C 490	-0.958 34.696 84.016 1.00 62.10	С
	5241 O MET C 490	-1.461 34.765 82.892 1.00 62.62	Ο
<b>ATOM</b>		1.490 34.790 84.308 1.00 60.35	С
<b>ATOM</b>	5243 CG MET C 490	2.660 35.639 83.837 1.00 60.29	С
		4.194 34.770 84.219 1.00 59.65	S
ATOM	5245 CE MET C 490	5.182 36.198 84.659 1.00 61.18	С
<b>ATOM</b>	5246 N ALA C 491	-1.349 33.800 84.920 1.00 62.86	N
		-2.451 32.878 84.664 1.00 62.45	С
		-3.679 33.758 84.502 1.00 63.52	С
		-4.366 33.675 83.486 1.00 64.88	Ο
		-2.617 31.907 85.793 1.00 61.59	С
		-3.908 34.692 85.425 1.00 64.00	N
			С
	5253 C LYS C 492		С
		-6.015 36.472 83.331 1.00 66.45	0
	5255 CB LYS C 492	-5.233 36.553 86.452 1.00 64.96	С
	5260 N ALA C 493		N
ATOM	5261 CA ALA C 493	-3.817 37.174 81.956 1.00 66.34	С
	5262 C ALA C 493	-4.062 36.093 80.910 1.00 66.80	C
	5263 O ALA C 493	-4.037 36.333 79.709 1.00 67.95	0
		-2.549 37.946 81.657 1.00 66.14	С
		-4.306 34.871 81.318 1.00 66.55	N
		-4.549 33.743 80.477 1.00 67.39	С
		-3.327 33.340 79.682 1.00 69.03	C
		-3.431 33.325 78.457 1.00 70.85	О
<b>ATOM</b>	5269 N LEUC 495	-2.156 33.035 80.240 1.00 69.12	N
		-1.042 32.605 79.401 1.00 67.66	С
	5271 C LEU C 495		C
	5272 O LEUC 495	-1.353 30.693 80.728 1.00 66.27	0
	5273 CB LEUC 495	0.326 33.123 79.765 1.00 67.67	C
	5274 CG LEU C 495		C
	5275 CD1 LEU C 495	2.030 34.891 80.136 1.00 67.69	C
	_	-0.128 35.456 78.998 1.00 69.10	C
	5277 N THR C 496	-0.644 30.323 78.648 1.00 67.85	N
	5278 CA THR C 496		C
	5279 C THR C 496	0.282 28.596 80.074 1.00 69.69	C
ATOM			0
ATOM	5281 CB THR C 496	0.131 28.249 77.679 1.00 69.65	С

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ATOM	5282	OG1 THR C 496	-0.649 28.629 76.549 1.00 70.83	0
		CG2 THR C 496	0.241 26.748 77.746 1.00 71.54	С
ATOM		N LEU C 497	0.243 27.387 80.603 1.00 70.09	N
ATOM		CA LEU C 497	1.104 26.974 81.695 1.00 70.17	С
ATOM		C LEU C 497	2.554 27.015 81.241 1.00 70.38	C
		O LEU C 497	3.468 27.257 82.022 1.00 70.44	0
		CB LEU C 497	0.734 25.569 82.077 1.00 71.33	C
ATOM		CG LEU C 497	0.560 25.185 83.533 1.00 72.65	C C
ATOM		CD1 LEU C 497	1.474 23.971 83.684 1.00 73.62 0.900 26.296 84.517 1.00 73.68	C
ATOM		CD2 LEU C 497 N GLN C 498	2.790 26.779 79.954 1.00 71.07	N
ATOM		CA GLN C 498	4.125 26.835 79.385 1.00 71.07	C
		C GLN C 498	4.522 28.281 79.136 1.00 69.80	c
		O GLN C 498	5.688 28.601 79.316 1.00 70.90	Ö
		CB GLN C 498	4.285 26.031 78.110 1.00 72.84	C
ATOM		CG GLN C 498	5.423 26.529 77.246 1.00 76.47	C
		CD GLN C 498	5.789 25.674 76.064 1.00 78.75	С
		OE1 GLN C 498	6.954 25.383 75.787 1.00 79.93	О
		NE2 GLN C 498	4.808 25.224 75.292 1.00 80.37	N
		N GLN C 499	3.637 29.190 78.769 1.00 68.09	N
		CA GLN C 499	4.045 30.579 78.566 1.00 66.52	C
		C GLN C 499	4.335 31.222 79.916 1.00 65.14	C
		O GLN C 499	5.128 32.156 80.000 1.00 65.15	O C
		CB GLN C 499	2.954 31.403 77.908 1.00 67.39 2.187 30.566 76.902 1.00 68.26	C
ATOM		CG GLN C 499 CD GLN C 499	1.351 31.474 76.031 1.00 69.04	Č
ATOM		OE1 GLN C 499	0.360 32.015 76.504 1.00 69.68	Ö
		NE2 GLN C 499	1.831 31.578 74.804 1.00 69.76	N
		N GLN C 500	3.651 30.693 80.931 1.00 62.78	N
		CA GLN C 500	3.837 31.173 82.288 1.00 60.68	С
		C GLN C 500	5.280 30.888 82.701 1.00 58.45	С
ATOM	5313	O GLN C 500	6.001 31.837 83.021 1.00 58.31	0
		CB GLN C 500	2.885 30.508 83.254 1.00 61.20	С
		CG GLN C 500	1.505 31.146 83.337 1.00 62.27	C
		CD GLN C 500	0.578 30.080 83.904 1.00 63.04	C
		OE1 GLN C 500	0.821 29.501 84.963 1.00 63.59	0
		NE2 GLN C 500	-0.480 29.815 83.175 1.00 63.65	N N
		N HIS C 501	5.709 29.635 82.623 1.00 55.31 7.082 29.352 83.006 1.00 53.62	C
		CA HIS C 501 C HIS C 501	8.090 30.065 82.126 1.00 53.32	c
		O HIS C 501	9.177 30.418 82.628 1.00 54.43	Ö
		CB HIS C 501	7.384 27.886 83.164 1.00 53.44	Č
			7.433 26.979 81.994 0.50 52.73	C
			6.349 27.013 83.805 0.50 53.70	C
		ND1AHIS C 501	6.855 25.722 82.044 0.50 52.67	N

WO"	98/5681	2	229/371	PCT/GB98/01708
ATOM	5372	CG AGLN C 506	10.997 35.027 79.008 0.50 49.22	С
ATOM	5373	CG BGLN C 506	10.997 35.027 79.008 0.50 49.22 11.982 35.439 78.402 0.50 47.09 10.287 35.261 77.712 0.50 50.52	С
ATOM	5374	CD AGLN C 506	10.287 35.261 77.712 0.50 50.52	С
ATOM	5375	CD BGLN C 506	13.443 35.396 78.009 0.50 47.98	С
ATOM	5376	OF LAGLN C 506	9.576 36.260 77.534 0.50 51.64	0
ATOM	5377	OE1BGLN C 506	14.172 36.371 78.271 0.50 49.11	0
ATOM	5378	NE2AGLN C 506	14.172 36.371 78.271 0.50 49.11 10.462 34.314 76.787 0.50 50.82	N
<b>ATOM</b>	5379	NE2BGLN C 506	13.898 34.308 77.392 0.50 46.84	N
ATOM	5380	N LEUC 507	11.595 37.106 82.794 1.00 47.02	N
ATOM	5381	CA LEU C 507	11.637 38.214 83.728 1.00 46.79	С
ATOM	5382	C LEU C 507	12,799 38,120 84,695 1.00 46,70	С
ATOM	5383	O LEUC 507	13.560 39.089 84.808 1.00 48.95	0_
ATOM	5384	CB LEU C 507	10.352 38.324 84.531 1.00 48.26	C
ATOM	5385	CG LEU C 507	9.117 38.715 83.712 1.00 49.58	C
ATOM	5386	CD1 LEU C 507	7.913 38.843 84.649 1.00 50.04	С
ATOM	5387	CD2 LEU C 507	9.362 40.006 82.960 1.00 49.77	C
ATOM	5388	N LEU C 508	12.972 37.000 85.367 1.00 45.26	N
ATOM	5389	CA LEU C 508	14.095 36.831 86.281 1.00 43.54 15.415 36.889 85.546 1.00 42.79	C C
ATOM	5390	C LEU C 508	15.415 35,889 85,346 1.00 42.79	0
ATOM	5391	O LEU C 508	16.349 37.442 86.161 1.00 44.62 13.903 35.535 87.070 1.00 43.30	
ATOM	5392	CB LEU C 508	12.574 35.493 87.827 1.00 42.75	
ATOM	5204	CD LEU C 508	12.432 34.160 88.525 1.00 45.27	c
ATOM	5305	CD1 LEU C 508	12.528 36.588 88.857 1.00 43.71	Č
ATOM	2306	N I ELL C 509	15.593 36.440 84.302 1.00 40.58	
			16.930 36.594 83.716 1.00 40.98	
ATOM	5398	C LEUC 509	17.371 38.056 83.559 1.00 41.80	
			18.571 38.373 83.557 1.00 40.85	
ATOM	5400	CB LEU C 509	17.133 35.825 82.417 1.00 39.19	С
ATOM	5401	CG LEU C 509	17.199 34.314 82.518 1.00 38.43	С
ATOM	5402	CDI LEU C 509	17.199 34.314 82.518 1.00 38.43 17.193 33.742 81.124 1.00 38.49	С
		CD2 LEU C 509	18.408 33.853 83.302 1.00 38.49	C
		N ILEC 510	16.437 39.005 83.446 1.00 42.22	N
<b>ATOM</b>	5405	CA ILE C 510	16.736 40.420 83.312 1.00 41.83	С
		C ILE C 510	17.415 40.875 84.591 1.00 41.01	С
		O ILEC 510	18.297 41.731 84.568 1.00 41.48	0
		CB ILE C 510	15.521 41.294 82.999 1.00 41.89	C
		CG1 ILE C 510	15.237 41.297 81.490 1.00 45.22	C
		CG2 ILE C 510	15.738 42.756 83.300 1.00 41.62	C
		CD1 ILE C 510	13.765 41.061 81.156 1.00 47.45	C
		N LEUC 511	17.034 40.302 85.721 1.00 40.64	N
		CA LEU C 511	17.645 40.700 86.982 1.00 41.72	C
		C LEUC511	19.161 40.571 86.924 1.00 42.18	C O
		O LEUC 511	19.883 41.400 87.487 1.00 43.39 17.051 39.931 88.151 1.00 41.42	C
ATOM	5416	CB LEU C 511	17.031 39.931 88.131 1.00 41.42	C

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ATOM	5417 CG LEU C 511	15.549 40.136 88.361 1.00 41.22	С
ATOM	5418 CD1 LEU C 511	15.186 39.555 89.731 1.00 41.54	С
ATOM	5419 CD2 LEU C 511	15.150 41.585 88.240 1.00 39.85	С
ATOM	5420 N SER C 512	19.719 39.597 86.239 1.00 41.63	N
<b>ATOM</b>	5421 CA SER C 512	21.143 39.455 86.122 1.00 41.44	C
<b>ATOM</b>	5422 C SER C 512	21.758 40.706 85.513 1.00 41.95	C
<b>ATOM</b>	5423 O SER C 512	22.722 41.284 86.035 1.00 42.95	0
<b>ATOM</b>	5424 CB SER C 512	21.414 38.338 85.114 1.00 43.11	С
		22.472 37.616 85.722 1.00 47.13	
		21.211 41.137 84.368 1.00 40.29	
<b>ATOM</b>	5427 CA HIS C 513	21.684 42.330 83.681 1.00 37.65	С
<b>ATOM</b>	5428 C HIS C 513	21.571 43.508 84.623 1.00 38.21	С
<b>ATOM</b>	5429 O HIS C 513	22.529 44.283 84.760 1.00 38.29	0
<b>ATOM</b>	5430 CB HIS C 513	20.913 42.523 82.391 1.00 37.61	С
ATOM	5431 CG AHIS C 513	21.265 41.340 81.520 0.50 38.24	C
ATOM	5432 CG BHIS C 513	21.461 43.588 81.495 0.50 39.47	C
ATOM	5433 ND1AHIS C 513	3 20.348 40.481 80.972 0.50 38.41	N
ATOM	5434 ND1BHIS C 513	3 20.716 44.626 80.974 0.50 39.63	N
ATOM	5435 CD2AHIS C 513	3 22.479 40.878 81.129 0.50 38.68	C
ATOM	5436 CD2BHIS C 513	3 22.721 43.759 80.999 0.50 40.24	
ATOM	5437 CE1AHIS C 513	20.978 39.547 80.280 0.50 38.17	
ATOM	5438 CE1BHIS C 513	21.484 45.382 80.212 0.50 40.30	C
ATOM	5439 NE2AHIS C 513	3 22.272 39.767 80.352 0.50 38.14	N
ATOM	5440 NE2BHIS C 513	22.716 44.877 80.208 0.50 40.60	N
ATOM	5441 N ILE C 514	20.451 43.655 85.332 1.00 37.46	N
ATOM	5442 CA ILE C 514	20.347 44.761 86.284 1.00 37.60	C C
		21.468 44.626 87.289 1.00 37.99	
ATOM	5444 O ILE C 514	22.180 45.604 87.576 1.00 38.56 18.949 44.788 86.900 1.00 38.83	c
			C
ATOM	5440 CGI ILE C 514	17.942 45.260 85.827 1.00 39.26 18.836 45.675 88.137 1.00 38.87	c
	5448 CD1 ILE C 514	16.544 44.724 86.101 1.00 37.40	Č
	5449 N ARG C 515	21.778 43.442 87.821 1.00 38.49	Ň
	5450 CA ARG C 515		Ċ
	5451 C ARG C 515	24.180 43.899 88.089 1.00 39.23	C
	5452 O ARG C 515		O
	5453 CB ARG C 515		C
	5454 CG ARG C 515		C
	5455 CD ARG C 515		С
	5456 NE ARG C 515		N
	5457 CZ ARG C 515		С
	5458 NH1 ARG C 51		N
	5459 NH2 ARG C 51		N
	5460 N HIS C 516	24.442 43.367 86.880 1.00 38.97	N
	5461 CA HIS C 516	25.559 43.743 86.079 1.00 37.57	С

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ATOM	5462 C HTS C 516	25.669 45.231 85.924 1.00 37.44	С
	5463 O HIS C 516		Ō
ATOM	5464 CB HIS C 516	25.484 43.088 84.675 1.00 39.10	С
		26.800 43.430 83.987 1.00 39.84	С
ATOM	5466 ND1 HIS C 516	28.000 42.830 84.270 1.00 38.68	N
ATOM	5467 CD2 HIS C 516	27.067 44.373 83.053 1.00 39.95	С
ATOM	5468 CE1 HIS C 516	28.926 43.374 83.556 1.00 38.48	С
		28.402 44.310 82.802 1.00 39.09	
	5470 N MET C 517		
	5471 CA MET C 517	24.581 47.349 85.315 1.00 41.49	С
ATOM	5472 C MET C 517	24.887 48.141 86.576 1.00 41.19	С
ATOM	5473 O MET C 517	25.656 49.088 86.572 1.00 40.45	0
ATOM	5474 CB MET C 517	23.133 47.749 84.952 1.00 42.86	C
ATOM	5475 CG MET C 517	23.062 48.179 83.500 1.00 44.59	C S
		21.375 48.400 82.948 1.00 45.13 20.821 46.716 83.021 1.00 47.50	C
	5477 CE MET C 517		N
	5478 N SER C 518	24.431 48.350 88.959 1.00 42.10	C .
	5480 C SER C 518		C
		26.435 49.226 89.972 1.00 40.04	Ö
ATOM	5482 CR SER C 518	23.515 47.681 89.976 1.00 43.27	C
ATOM	5483 OG SER C 518	24.029 47.552 91.289 1.00 44.28	Ö
		26.559 47.178 89.096 1.00 42.60	N
ATOM	5485 CA ASN C 519	27.949 46.967 89.451 1.00 44.06	С
	5486 C ASN C 519		С
ATOM	5487 O ASN C 519	29.549 48.667 89.315 1.00 47.80	0
		28.448 45.555 89.206 1.00 45.80	C
ATOM	5489 CG ASN C 519	28.018 44.580 90.279 1.00 47.88	C
		27.926 45.010 91.435 1.00 50.31	0
	5491 ND2 ASN C 519		N
ATOM	5492 N LYS C 520	28.523 48.167 87.396 1.00 45.89	N C
	5493 CA LYS.C 520	29,236 49.176 86.629 1.00 46.46 28.835 50.560 87.130 1.00 46.04	C
	5494 C LYS C 520	29.666 51.452 87.255 1.00 47.08	0
	5495 O LYS C 520 5496 CB LYS C 520	28.836 49.062 85.154 1.00 48.75	C
	5497 CG LYS C 520	28.821 47.585 84.751 1.00 50.92	C ·
	5498 CD LYS C 520	30.184 47.325 84.145 1.00 53.90	Č
	5499 CE LYS C 520	31.038 46.337 84.914 1.00 55.45	Č
	5500 NZ LYS C 520	32.449 46.457 84.423 1.00 57.07	N
	5501 N GLY C 521	27.558 50.761 87.425 1.00 44.57	N
	5502 CA GLY C 521	27.144 52.049 87.936 1.00 44.81	С
	5503 C GLY C 521	27.929 52.417 89.189 1.00 45.01	С
	5504 O GLY C 521	28.386 53.562 89.186 1.00 45.65	О
	5505 N MET C 522	28.095 51.592 90.230 1.00 45.15	N
ATOM	5506 CA MET C 522	28.807 52.064 91.396 1.00 46.35	С

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	6507 C MET C 500	252 (37)	
		30.253 52.370 90.993 1.00 <b>48.58</b> 30.785 53.372 91.449 1.00 <b>49.59</b>	C O
		29.054 51.248 92.623 1.00 46.05	
		28.178 50.220 93.195 1.00 47.14	
ATOM	5511 SD MET C 522	26,835 50,822 94,200 1,00 48,30	S
ATOM	5512 CE MET C 522	26.835 50.822 94.200 1.00 48.30 27.488 52.344 94.834 1.00 47.03	С
		30.839 51.485 90.186 1.00 50.74	
		32.219 51.708 89.771 1.00 50.96	
		32.345 53.103 89.211 1.00 47.76	
		33.253 53.809 89.603 1.00 47.73	0
		32.667 50.627 88.824 1.00 56.55	
ATOM	5518 CG GLU C 523	33.327 49.441 89.503 1.00 64.56	C
ATOM	5519 CD GLU C 523	34.430 49.763 90.500 1.00 69.18	С
ATOM	5520 OE1 GLU C 523	34.979 50.901 90.485 1.00 71.53 34.775 48.861 91.321 1.00 71.46	0
		31.443 53.541 88.377 1.00 45.46	N
		31.422 54.860 87.801 1.00 45.10	C
		31.139 55.989 88.775 1.00 45.54	c
		31.760 57.047 88.813 1.00 43.84	Ö
		30.302 54.867 86.714 1.00 44.35	
ATOM	5527 CG HIS C 524	30.172 56.201 86.043 1.00 43.95	С
<b>ATOM</b>	5528 ND1 HIS C 524	29.392 57.207 86.582 1.00 44.66	N
<b>ATOM</b>	5529 CD2 HIS C 524	30.702 56.715 84.921 1.00 43.61	С
		29.451 58.282 85.815 1.00 44.69	
		30.246 58.006 84.791 1.00 44.31	
		30.129 55.837 89.635 1.00 47.24	
		29.737 56.875 90.572 1.00 49.14	
		30.940 57.158 91.461 1.00 52.11	
ATOM	5535 O LEU C 525	31.220 58.281 91.867 1.00 52.94	0
ATOM	5536 CB LEU C 525	28.524 56.521 91.430 1.00 47.83 28.177 57.531 92.529 1.00 46.65	C C
	5537 CG LEU C 525 5538 CD1 LEU C 525	27.759 58.851 91.904 1.00 46.66	C
	5539 CD2 LEU C 525		C
	5540 N TYR C 526	31.622 56.068 91.767 1.00 54.77	N
	5541 CA TYR C 526	32.813 56.096 92.574 1.00 57.68	C
	5542 C TYR C 526	33,902 56.853 91.852 1.00 58.29	C
	5543 O TYR C 526	34.445 57.709 92.533 1.00 59.72	O
<b>ATOM</b>	5544 CB TYR C 526	33.217 54.646 92.801 1.00 61.45	C
	5545 CG TYR C 526		C
	5546 CD1 TYR C 526		C
	5547 CD2 TYR C 526		C
	5548 CE1 TYR C 526		C
	5549 CE2 TYR C 526	36.771 54.443 94.040 1.00 68.71	C
	5550 CZ TYR C 526		C
ATOM	5551 OH TYRC 526	37.667 54.593 96.230 1.00 74.04	O

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		234/371	
		33.576 65.532 91.235 1.00 85.41	
		32.575 66.043 90.328 1.00 83.84	C
		31.192 65.917 90.966 1.00 84.07	C
		30.192 66.581 90.690 1.00 <b>85</b> .18 32.587 65.178 89.053 1.00 <b>83</b> .29	O C
ATOM	5604 CG1 VAL C 533	31.687 65.744 87.979 1.00 83.42	C
ATOM	5605 CG2 VAL C 533	33.980 64.923 88.521 1.00 82.88	C
		31.094 64.963 91.882 1.00 83.18	N
		29.895 64.631 92.612 1.00 82.16	
		29.866 65.401 93.925 1.00 81.49	C
		30.817 65.427 94.693 1.00 80.19	0
<b>ATOM</b>	5610 CB VAL C 534	29.905 63.124 92.979 1.00 83.14	С
<b>ATOM</b>	5611 CG1 VAL C 534	28.769 62.657 93.896 1.00 82.66	С
		29.879 62.310 91.680 1.00 83.87	С
	5613 N PRO C 535		N
		28.413 66.702 95.382 1.00 82.22	С
	5615 C PRO C 535		C
		28.315 64.471 96.489 1.00 82.55	0
		27.037 67.375 95.227 1.00 81.89	C
		26.639 67.049 93.824 1.00 81.50 27.549 65.969 93.280 1.00 81.99	
	5620 N LEUC 536		N
	5621 CA LEU C 536	28.458 65.656 99.010 1.00 85.26	C
	5622 C LEU C 536		<del>=</del>
	5623 O LEU C 536		O
	5628 N TYR C 537		N
		24.946 64.232 99.320 1.00 78.85	С
		25.325 63.093 100.266 1.00 76.77	С
ATOM	5631 O TYR C 537	26.030 62.171 99.878 1.00 75.21	0
ATOM	5632 CB TYR C 537	23.950 63.823 98.270 1.00 79.38	C
	5633 CG TYR C 537	23.674 64.920 97.266 1.00 80.32	C
	5634 CD1 TYR C 537	23.077 66.101 97.666 1.00 80.91	C
		23.998 64.786 95.923 1.00 80.96	C
	5636 CE1 TYR C 537	22.810 67.113 96.765 1.00 81.66	C C
	5637 CE2 TYR C 537 5638 CZ TYR C 537	23.725 65.799 95.029 1.00 81.20 23.135 66.962 95.437 1.00 81.56	C
	5639 OH TYR C 537	22.870 67.969 94.533 1.00 82.05	0
	5640 N ASP C 538	24.878 63.218 101.503 1.00 75.21	N
	5641 CA ASP C 538	25.123 62.267 102.558 1.00 72.00	C
	5642 C ASP C 538	24.514 60.891 102.464 1.00 66.75	c
	5643 O ASP C 538	25.237 59.938 102.741 1.00 65.15	Ö
	5644 CB ASP C 538	24.546 62.905 103.842 1.00 77.25	C
	5645 CG ASP C 538	25.685 63.756 104.406 1.00 82.29	С
ATOM	5646 OD1 ASP C 538	26.854 63.294 104.279 1.00 84.32	0
ATOM	5647 OD2 ASP C 538	25.382 64.854 104.952 1.00 85.06	0

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	2 <i>36/37</i> 4	
OM 5603 CR LETT 544	28 520 55 356 97 268 1 00 50 22	C

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ATOM	5693	CB LEU C 544	28.529 55.356 97.268 1.00 50.22	С
ATOM	5694	CG LEU C 544	29.858 55.297 96.534 1.00 49.15	С
ATOM	5695	CD1 LEU C 544	29.894 54.324 95.377 1.00 48.25	С
ATOM	5696	CD2 LEU C 544	30.186 56.690 96.017 1.00 49.91	С
ATOM	5697	N ASP C 545	29.385 53.991 100.025 1.00 55.73	N
ATOM		CA ASP C 545	30.407 53.413 100.875 1.00 59.57	С
ATOM	5699	C ASP C 545	30.082 51.990 101.298 1.00 59.45	С
ATOM	5700	O ASP C 545	31.051 51.236 101.382 1.00 59.14	0
ATOM	5701	CB ASP C 545	30.688 54.156 102.167 1.00 64.30	С
<b>ATOM</b>	5702	CG ASP C 545	31.229 55.548 101.904 1.00 69.40	С
ATOM	5703	OD1 ASP C 545	31.653 55.841 100.746 1.00 71.67	Ο
ATOM		OD2 ASP C 545	31.204 56.334 102.902 1.00 71.66	0
ATOM	5705	N ALA C 546	28.827 51.628 101.525 1.00 59.48	N
ATOM	5706	CA ALA C 546	28.511 50.253 101.878 1.00 60.67	C
ATOM	5707	C ALA C 546	29.213 49.276 100.938 1.00 63.24	С
ATOM	5708	O ALA C 546	29.817 48.285 101.346 1.00 63.11	Ο
ATOM	5709	CB ALA C 546	27.021 50.031 101.782 1.00 60.55	С
ATOM	5710	N HIS C 547	29.145 49.528 99.636 1.00 66.39	N
ATOM	5711	CA HIS C 547	29.733 48.761 98.582 1.00 68.73	С
<b>ATOM</b>	5712	C HIS C 547	31.229 48.744 98.582 1.00 73.05	С
ATOM	5713	O HIS C 547	31.804 47.671 98.445 1.00 74.71	Ο
<b>ATOM</b>	5714	CB HIS C 547	29.306 49.374 97.221 1.00 66.98	С
ATOM	5715	CG HIS C 547	27.919 48.813 97.109 1.00 65.98	С
ATOM	5716	ND1 HIS C 547	27.619 47.765 96.300 1.00 66.00	N
<b>ATOM</b>	5717	CD2 HIS C 547	26.791 49.151 97.760 1.00 66.17	С
<b>ATOM</b>	5718	CE1 HIS C 547	26.334 47.482 96.431 1.00 66.20	С
ATOM	5719	NE2 HIS C 547	25.809 48.302 97.307 1.00 66.22	N
ATOM	5720	N ARG C 548	31.838 49.906 98.715 1.00 78.91	N
<b>ATOM</b>	5721	CA ARG C 548	33.320 49.931 98.704 1.00 84.25	С
<b>ATOM</b>	5722	C ARG C 548	33.895 49.165 99.889 1.00 84.99	С
ATOM	5723	O ARG C 548	33.110 48.818 100.817 1.00 86.30	0
<b>ATOM</b>	5724	CB ARG C 548	33.796 51.385 98.630 1.00 87.34	С
<b>ATOM</b>	5725	CG ARG C 548	32.949 52.389 97.863 1.00 89.98	С
<b>ATOM</b>	5726	CD ARG C 548	32.592 52.060 96.435 1.00 92.13	С
ATOM	5727	NE ARG C 548		N
<b>ATOM</b>	5728	CZ ARG C 548	33.197 50.465 94.601 1.00 95.46	С
<b>ATOM</b>	5729	NH1 ARG C 548	32.046 50.556 93.960 1.00 96.52	N
<b>ATOM</b>	5730	NH2 ARG C 548	34.109 49.668 94.075 1.00 96.02	N
TER 5	731	ARG C 548		
HETAT	M 573	2 C1 EST C 600	19.869 58.501 89.282 1.00 35.71	С
HETAT	M 573	3 C2 EST C 600	18.524 58.409 89.623 1.00 37.42	С
HETAT	M 573	4 C3 EST C 600	17.822 57.308 89.220 1.00 38.32	С
HETAT	M 573	5 O3 EST C 600	16.483 57.175 89.546 1.00 38.91	Ο
		6 C4 EST C 600		С
HETAT	M 573	7 C5 EST C 600	19.774 56.391 88.128 1.00 36.82	С

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HETATM 5738 C6 EST C 600 HETATM 5739 C7 EST C 600	20.294 55.421 87.091 1.00 37.10 21.704 55.728 86.604 1.00 36.50	C
HETATM 5740 C8 EST C 600		č
HETATM 5741 C9 EST C 600		č
HETATM 5742 C10 EST C 600	20.489 57.499 88.548 1.00 35.28	
	22.728 58.299 89.298 1.00 35.64	
HETATM 5744 C12 EST C 600		С
HETATM 5745 C13 EST C 600	24.772 57.250 88.396 1.00 35.67	
	23.932 56.551 87.306 1.00 35.16	
HETATM 5747 C15 EST C 600	24.852 55.358 87.058 1.00 35.36	C
HETATM 5748 C16 EST C 600	26.207 56.101 86.772 1.00 36.43	C
HETATM 5749 C17 EST C 600	26.129 57.338 87.694 1.00 36.25	C
HETATM 5750 O17 EST C 600	27.295 57.444 88.500 1.00 35.57	0
HETATM 5751 C18 EST C 600	24.895 56.358 89.623 1.00 35.57	C
ATOM 5752 N SER D 305	17.263 25.806 62.987 1.00 89.17	N C
ATOM 5/53 CA SER D 305	18.225 25.610 64.101 1.00 88.43 17.959 24.319 64.864 1.00 87.99	C
	16.871 24.093 65.388 1.00 87.53	0
ATOM 5756 CR SEP D 305	18.202 26.835 65.025 1.00 88.28	C
ATOM 5757 OG SER D 305	19.076 26.687 66.122 1.00 88.48	Ö
ATOM 5757 OG SEKED 306	18.986 23.473 64.970 1.00 87.77	N
ATOM 5759 CA LEU D 306	18.892 22.224 65.722 1.00 87.21	С
ATOM 5760 C LEU D 306		С
ATOM 5761 O LEU D 306	17.265 22.095 67.508 1.00 85.96	0
ATOM 5762 CB LEU D 306	20.260 21.563 65.896 1.00 87.76	C
ATOM 5766 N ALA D 307	18.916 23.530 67.764 1.00 83.98	N
ATOM 5767 CA ALA D 307	18.454 24.030 69.037 1.00 82.92	С
ATOM 5768 C ALA D 307	16.936 23.984 69.095 1.00 81.76	C
ATOM 5769 O ALA D 307	16.381 23.264 69.911 1.00 81.64	O C
	18.859 25.491 69.224 1.00 83.73 16.268 24.720 68.224 1.00 81.06	N
ATOM 5771 N LEU D 308	14.821 24.770 68.211 1.00 80.81	C
ATOM 5772 CA LEU D 308		c
ATOM 5774 O LEU D 308		Ō
ATOM 5775 CB LEU D 308	14.399 25.920 67.280 1.00 80.70	С
ATOM 5776 CG LEU D 308		С
ATOM 5777 CD1 LEU D 308	14.130 28.397 66.971 1.00 81.19	C
ATOM 5778 CD2 LEU D 308	14.940 27.533 69.155 1.00 81.20	С
ATOM 5779 N SER D 309	14.715 22.378 67.525 1.00 80.53	N
ATOM 5780 CA SER D 309	14.075 21.138 67.169 1.00 79.50	С
ATOM 5781 C SER D 309	14.253 20.044 68.198 1.00 78.69	C
ATOM 5782 O SER D 309	13.378 19.186 68.319 1.00 79.89 14.740 20.609 65.891 1.00 80.73	O C
ATOM 5783 CB SER D 309		0
ATOM 5784 OG SER D 309 ATOM 5785 N LEU D 310		N
ATOM 3/03 IN LEU D 310	13.303 20.021 00.902 1.00 10.10	4.1

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АТОМ	5786 CA LEUD 310	15.586 18.976 69.894 1.00 74.02	С
		14.459 19.034 70.927 1.00 72.78	
		13.795 20.037 71.154 1.00 72.43	0
ATOM	5789 CB LEUD 310	16.950 19.048 70.540 1.00 73.54	
ATOM	5790 CG LEUD 310	18.073 19.617 69.677 1.00 72.90	С
ATOM	5791 CD1 LEU D 310	18.593 20.870 70.346 1.00 <b>73</b> .00 19.183 18.589 69.545 1.00 <b>73</b> .78	C
ATOM	5792 CD2 LEU D 310	19.183 18.589 69.545 1.00 73.78	C
		14.248 17.880 71.528 1.00 71.14 13.223 17.687 72.536 1.00 69.71	
ATOM	5795 C. THR D 311	13.896 17.914 73.860 1.00 69.14	C C
ATOM	5796 O THR D 311	15.114 17.705 73.880 1.00 69.46	
		12.696 16.259 72.386 1.00 70.04	
<b>ATOM</b>	5798 OG1 THR D 311	13.681 15.274 72.691 1.00 69.74	0
ATOM	5799 CG2 THR D 311	12.246 16.024 70.952 1.00 69.87	С
		13.215 18.263 74.934 1.00 68.71	N
		13.912 18.480 76.198 1.00 68.63	
ATOM	5802 C ALA D 312	14.925 17.380 76.447 1.00 68.98 16.044 17.697 76.851 1.00 69.24	
		12.983 18.641 77.366 1.00 68.89	O C
		14.592 16.129 76.206 1.00 70.40	
		15.559 15.061 76.417 1.00 72.08	
<b>ATOM</b>	5807 C ASP D 313	16.794 15.157 75.562 1.00 69.74	c
<b>ATOM</b>	5808 O ASP D 313	16.794 15.157 75.562 1.00 69.74 17.855 14.913 76.108 1.00 68.84	0
ATOM	5809 CB ASP D 313	14.902 13.680 76.231 1.00 76.64	С
ATOM	5810 CG ASP D 313	14.055 13.442 77.472 1.00 80.32	С
ATOM	5811 OD1 ASP D 313	14.677 13.473 78.554 1.00 82.36 12.822 13.267 77.370 1.00 82.59	0
ATOM	5812 VD2 ASP D 313	12.822 13.267 77.370 1.00 82.59	0
		16.722 15.478 74.298 1.00 69.16 17.892 15.578 73.433 1.00 69.14	
		18.762 16.748 73.860 1.00 67.43	C .
		19.983 16.632 73.906 1.00 67.85	0
	5817 CB GLN D 314	17.494 15.775 71.972 1.00 71.65	C
ATOM	5818 CG GLN D 314	16.256 14.951 71.631 1.00 74.11	С
	5819 CD GLN D 314	15.887 15.055 70.179 1.00 76.25	С
	5820 OE1 GLN D 314	14.964 15.747 69.756 1.00 77.94	0
	5821 NE2 GLN D 314 5822 N MET D 315	16.681 14.318 69.406 1.00 77.91	N
	5823 CA MET D 315	18.104 17.860 74.181 1.00 64.64 18.765 19.058 74.684 1.00 60.92	N C
	5824 C MET D 315	19.646 18.678 75.867 1.00 58.71	C
	5825 O MET D 315	20.853 18.867 75.830 1.00 57.58	O
	5826 CB MET D 315	17.704 20.050 75.130 1.00 60.65	C
	5827 CG MET D 315	18.233 21.397 75.579 1.00 61.16	С
	5828 SD MET D 315	18.673 22.508 74.236 1.00 60.09	S
	5829 CE MET D 315	20.398 22.700 74.561 1.00 60.98	C
ATOM	5830 N VAL D 316	19.068 18.104 76.912 1.00 57.26	N

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4 TO 3 (	5021 CA WAI D 214	27 (707) 10 912 17 697 79 077 1 00 57 09	С
ATOM	5831 CA VALD 316	19.812 17.687 78.077 1.00 57.08	c
		21.023 16.839 77.740 1.00 58.01 22.096 17.031 78.310 1.00 58.94	0
		18.988 16.858 79.081 1.00 56.33	
ATOM	5834 CB VALD 316	19.824 16.374 80.254 1.00 55.69	C
ATOM	5934 CG2 VAL D 316	17.844 17.705 79.587 1.00 56.75	C
		20.878 15.857 76.879 1.00 59.33	
		21.985 14.964 76.529 1.00 60.63	
ATOM	5830 C SEP D 317	23.029 15.693 75.710 1.00 58.92	
ATOM	5840 O SER D 317	24.220 15.563 75.947 1.00 59.22	Ö
		21.463 13.769 75.722 1.00 62.99	
ATOM	5842 OG SER D 317	20.092 14.067 75.446 1.00.66.00	
ATOM	5843 N ALA D 318	20.092 14.067 75.446 1.00 66.00 22.565 16.502 74.770 1.00 57.14	N
ATOM	5844 CA ALAD 318	23.496 17.287 73.969 1.00 55.70	C
ATOM	5845 C ALA D 318	24.400 18.069 74.923 1.00 55.38	C ·
		25.619 18.111 74.754 1.00 55.90	
ATOM	5847 CB ALA D 318	22.719 18.241 73.089 1.00 55.59	C
		23.784 18.710 75.917 1.00 54.11	
		24.469 19.510 76.902 1.00 52.31	
ATOM	5850 C LEU D 319	25.325 18.635 77.770 1.00 53.63	
ATOM	5851 O LEU D 319	26.487 18.939 77.974 1.00 53.68	0
ATOM	5852 CB LEU D 319	23.447 20.269 77.728 1.00 50.38	С
		22.730 21.396 76.981 1.00 48.85	
ATOM	5854 CD1 LEU D 319	21.761 22.043 77.948 1.00 48.88	C
		23.707 22.414 76.424 1.00 48.75	С
		24.790 17.509 78.221 1.00 55.98	N
		25.548 16.575 79.053 1.00 57.36	
ATOM	5858 C LEU D 320	26.763 16.093 78.304 1.00 60.13	С
ATOM	5859 O LEU D 320	27.824 15.833 78.843 1.00 62.13	0
ATOM	5860 CB LEU D 320	24.641 15.409 79.440 1.00 56.38	C
		23.973 15.674 80.783 1.00 56.64	С
	5862 CD1 LEU D 320	23.038 14.548 81.152 1.00 56.78	C
	5863 CD2 LEU D 320	25.048 15.937 81.831 1.00 56.47	C
	5864 N ASP D 321	26.669 15.954 77.004 1.00 63.24	N
	5865 CA ASP D 321	27.748 15.558 76.161 1.00 66.90	C
	5866 C ASP D 321	28.809 16.606 75.920 1.00 66.24	С
	5867 O ASP D 321	29.986 16.236 75.844 1.00 68.96	0
	5868 CB ASP D 321	27.206 15.266 74.754 1.00 72.33 27.150 13.752 74.641 1.00 77.63	C
	5869 CG ASP D 321 5870 OD1 ASP D 321	27.464 13.085 75.664 1.00 80.31	0
	5871 OD2 ASP D 321	26.783 13.313 73.522 1.00 80.62	o
	5872 N ALA D 322	28.452 17.873 75.776 1.00 62.64	N
	5873 CA ALA D 322	29.463 18.891 75.524 1.00 58.96	C
	5874 C ALA D 322	30.353 19.113 76.735 1.00 58.25	C ×-
	5875 O ALA D 322	31.386 19.785 76.571 1.00 58.76	Ö
711 OIVI	30.3 O ALA D 322	31.556 17.765 76.571 1.66 56.76	<del>-</del>

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		240/371	
		28.714 20.137 75.123 1.00 57.92	
		30.011 18.611 77.925 1.00 55.35	
ATOM	5878 CA GLU D 323	30.845 18.879 79.074 1.00 54.74	C
ATOM	5879 C GLU D 323	32.304 18.681 78.796 1.00 55.52 32.712 17.725 78.133 1.00 59.31	
ATOM	5880 O GLUD 323	32.712 17.725 /8.133 1.00 59.31	O C
ATOM	5881 CB GLUD 323	30.312 18.010 80.193 1.00 54.82	
ATOM	5882 CG GLUD 323	29.099 18.698 80.835 1.00 55.81	
ATOM	5883 CD GLUD 323	29.559 19.859 81.695 1.00 56.08 30.318 19.628 82.658 1.00 56.53	0
ATOM	5884 OE1 GLU D 323	20.104.21.000.81.280.1.00.56.04	0
ATOM	5885 UEZ GLU D 323	29.194 21.000 81.389 1.00 56.04 33.174 19.567 79.226 1.00 54.31	
ATOM	5007 CA DDOD 324	34.603 19.489 79.046 1.00 53.97	C
ATOM	5000 C DDO D 224	35.190 18.524 80.065 1.00 54.99	c
ATOM	5000 O DDOD 324	34.527 18.093 81.003 1.00 55.95	Ö
ATOM	5800 CR DROD 324	35.145 20.897 79.323 1.00 53.50	
ATOM	5801 CG PROD 324	34 116 21 300 80 280 1 00 53 81	Č
ATOM	5802 CD PROD 324	34.116 21.390 80.280 1.00 53.81 32.788 20.736 80.013 1.00 54.57	Č
ATOM	5892 CD TROD 325	36.446 18.172 79.897 1.00 55.53	N
		37.181 17.283 80.757 1.00 56.14	
ATOM	5895 C PRO D 325	37 550 18 011 82 030 1.00 57.89	C
ATOM	5896 O PRO D 325	37.550 18.011 82.030 1.00 57.89 37.570 19.230 81.928 1.00 58.94	Ō
ATOM	5897 CB PRO D 325	38.475 16.991 79.994 1.00 56.36	C
		38.641 18.258 79.193 1.00 56.53	
ATOM	5899 CD PRO D 325	37.258 18.691 78.774 1.00 56.29	С
<b>ATOM</b>	5900 N ILE D 326	37.844 17.373 83.144 1.00 60.27	N
ATOM	5901 CA ILE D 326	38.234 18.094 84.359 1.00 62.33	С
ATOM	5902 C ILE D 326	39.764 18.203 84.337 1.00 60.55	С
ATOM	5903 O ILE D 326	40.396 17.168 84.156 1.00 60.17	0
ATOM	5904 CB ILE D 326	37.862 17.459 85.718 1.00 64.81	C
		38.409 16.036 85.871 1.00 66.11	C
		36.355 17.465 86.018 1.00 64.84	C
		38.045 15.056 84.781 1.00 67.42	C
		40.333 19.374 84.487 1.00 59.44	N
	5909 CA LEU D 327	41.786 19.485 84.472 1.00 58.05	C
	5910 C LEU D 327		C
	5911 O LEUD 327	41.603 19.137 86.848 1.00 58.48	0
	5912 CB LEU D 327	42.181 20.876 83.979 1.00 57.02	C C
	5913 CG LEU D 327	41.514 21.360 82.693 1.00 55.77	C
	5914 CD1 LEU D 327	42.331 22.494 82.103 1.00 55.92 41.316 20.258 81.683 1.00 54.67	C
	5915 CD2 LEU D 327 5916 N TYR D 328	43.625 19.048 85.975 1.00 60.29	N
	5916 N 1 1 R D 328	44.309 18.821 87.228 1.00 61.30	C
	5917 CA TTR D 328	45.235 20.026 87.385 1.00 61.97	C
	5919 O TYR D 328	45.706 20.500 86.372 1.00 60.71	Ö
	5920 CB TYR D 328		C
121 O1VI	5,20 CD 111CD 520	.5.1,5 1565 07.2.15 1.00 02.10	-

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ATOM	5921 CG TYR D 328		С
		43.836 16.059 88.678 1.00 64.19	
		43.876 15.593 86.339 1.00 62.75	С
		42.988 15.002 88.813 1.00 64.91	С
		43.040 14.504 86.495 1.00 63.95	
		42.598 14.208 87.761 1.00 65.57	
		41.757 13.126 87.962 1.00 67.54	
		45.439 20.471 88.599 1.00 64.59	N
		46.299 21.612 88.807 1.00 67.29	C C
	5930 C SER D 329	47.740 21.149 88.595 1.00 70.20 48.045 20.027 88.947 1.00 69.65	0
		46.144 22.172 90.214 1.00 66.33	
		47.308 22.949 90.451 1.00 66.37	
		48.571 22.000 88.029 1.00 74.75	
ATOM	5935 CA GLUD 330	49.973 21.777 87.782 1.00 78.76	C
		50.689 21.590 89.127 1.00 80.31	С
		50.542 22.260 90.146 1.00 80.76	
ATOM	5938 CB GLU D 330	50.572 22.972 87.056 1.00 82.49	С
ATOM	5939 CG GLUD 330	51.622 23.768 87.798 1.00 88.02	C
		51.312 25.158 88.310 1.00 91.02	С
		51.356 26.143 87.516 1.00 92.36	
		51.036 25.301 89.529 1.00 92.28 52.571 28.436 99.492 1.00 85.53	O N
		51.517 29.299 98.999 1.00 84.78	C
		51.805 30.749 99.360 1.00 83.45	
		51.984 31.023 100.540 1.00 84.23	
ATOM	5948 CG PHE D 337	50.138 28.994 99.593 1.00 85.69 49.414 27.933 98.825 1.00 86.82	С
ATOM	5949 CD1 PHE D 337	49.653 27.716 97.485 1.00 87.53	С
ATOM	5950 CD2 PHE D 337	48.492 27.138 99.467 1.00 87.80	C
		48.988 26.725 96.804 1.00 88.56	C
	5952 CE2 PHE D 337	47.808 26.143 98.802 1.00 88.39	C - ·
	5953 CZ PHE D 337 5954 N SER D 338	48.060 25.940 97.460 1.00 88.89 51.811 31.600 98.360 1.00 80.74	C N
	5955 CA SER D 338	52.050 33.020 98.634 1.00 77.84	C
	5956 C SER D 338	51.096 33.751 97.717 1.00 75.96	c
	5957 O SER D 338	50.725 33.148 96.709 1.00 76.63	Ö
	5958 CB SER D 338	53.489 33.358 98.294 1.00 77.31	C
	5959 OG SER D 338	53.793 32.794 97.042 1.00 77.40	0
	5960 N GLUD 339	50.740 34.984 97.978 1.00 73.50	N
	5961 CA GLU D 339	49.848 35.681 97.047 1.00 71.53	С
	5962 C GLU D 339	50.264 35.297 95.634 1.00 69.88	C
	5963 O GLUD 339	49.482 34.729 94.879 1.00 69.90	0
	5964 CB GLUD 339	49.905 37.153 97.342 1.00 71.56	C
AIUM	5965 CG GLU D 339	49.622 38.158 96.250 1.00 72.26	C

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4 mo> 4	tott op Gill Dage	242/371	0
ATOM	5966 CD GLUD 339	49.019 39.364 96.939 1.00 <b>73</b> .84 48.099 39.104 97.747 1.00 <b>74</b> .71	0
ATOM	2001 OEI GLU D 339	49.466 40.503 96.691 1.00 75.27	0
		51.503 35.551 95.251 1.00 68.32	
ATOM	5970 CA ALAD 340	51.964 35.211 93.926 1.00 66.84	С
ATOM	5971 C ALA D 340	51.857 33.743 93.572 1.00 65.40	C
ATOM	5972 O ALA D 340	51.426 33.462 92.464 1.00 65.53	0
<b>ATOM</b>	5973 CB ALA D 340	53.428 35.594 93.817 1.00 68.19	С
<b>ATOM</b>	5974 N SER D 341	52.278 32.843 94.438 1.00 64.29	N
		52.224 31.429 94.117 1.00 63.99	
		50.790 30.981 93.942 1.00 63.79	
ATOM	5977 O SER D 341	50.499 30.238 92.997 1.00 65.43	0
ATOM	5978 CB SER D 341	52.954 30.602 95.145 1.00 65.29 52.117 20.756 05.800 1.00.66.80	C
ATOM	39/9 OG 3EKD 341	32.117 29.730 93.890 1.00 00.80	U
		49.868 31.390 94.800 1.00 62.43	
		48.477 31.005 94.670 1.00 60.24 47.790 31.641 93.472 1.00 58.97	
		47.111 30.947 92.714 1.00 60.15 47.632 31.381 95.885 1.00 60.40	
		46.340 30.569 95.771 1.00 60.77	
ATOM	5986 SD MET D 342	45 537 30 453 97 364 1 00 61 98	Š
ATOM	5987 CE MET D 342	45.537 30.453 97.364 1.00 61.98 45.044 32.154 97.570 1.00 61.13	Č
		47.943 32.936 93.235 1.00 56.72	
		47.372 33.564 92.053 1.00 54.94	
ATOM	5990 C MET D 343	47.886 32.813 90.835 1.00 54.84	С
ATOM	5991 O MET D 343	47.107 32.531 89.932 1.00 56.41	0
		47.725 35.027 91.899 1.00 54.20	
		46.877 35.829 92.890 1.00 54.05	
ATOM	5994 SD MET D 343	45.115 35.671 92.551 1.00 51.49	S
		45.079 35.840 90.775 1.00 52.48	
	5996 N GLY D 344		N
		49.655 31.667 89.709 1.00 52.12	C
		48.854 30.395 89.497 1.00 51.85 48.396 30.211 88.372 1.00 52.11	C O
		48.658 29.497 90.457 1.00 51.64	N
	6001 CA LEU D 345	47.931 28.273 90.199 1.00 52.00	Č
	6002 C LEU D 345	46.528 28.472 89.651 1.00 51.27	c
	6003 O LEU D 345	46.087 27.901 88.665 1.00 51.16	Ö
	6004 CB LEU D 345	47.632 27.522 91.490 1.00 54.64	С
		48.809 26.826 92.152 1.00 57.14	С
		48.899 27.410 93.558 1.00 58.00	C
<b>ATOM</b>	6007 CD2 LEU D 345	48.609 25.316 92.126 1.00 57.34	С
	6008 N LEUD 346	45.815 29.290 90.432 1.00 49.48	N
	6009 CA LEU D 346	44.426 29.633 90.113 1.00 46.93	C
ATOM	6010 C LEU D 346	44.321 30.166 88.701 1.00 45.54	С

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ATOM	6011	O LEU D 346	43.616 29.725 87.814 1.00 43.40	О
ATOM	6012	CB LEUD 346	44.053 30.607 91.219 1.00 46.39	С
<b>ATOM</b>	6013	CG LEU D 346	43.730 29.934 92.553 1.00 46.28	С
<b>ATOM</b>	6014	CD1 LEU D 346	42.954 30.921 93.427 1.00 47.05	С
<b>ATOM</b>	6015	CD2 LEU D 346	42,957 28,648 92,439 1.00 44.06	С
<b>ATOM</b>	6016	N THR D 347	45.136 31.171 88.432 1.00 45.12	N
<b>ATOM</b>	6017	CA THR D 347	45.245 31.813 87.130 1.00 44.75	С
<b>ATOM</b>	6018	C THR D 347	45.663 30.858 86.058 1.00 44.99	C
ATOM	6019	O THR D 347	45.116 30.886 84.965 1.00 46.02	0
			46.194 32.989 87.399 1.00 44.97	С
<b>ATOM</b>	6021	OG1 THR D 347	45.363 34.166 87.260 1.00 46.54	0
ATOM	6022	CG2 THR D 347	47.482 32.992 86.660 1.00 43.19	С
ATOM	6023	N ASN D 348	46.589 29.951 86.286 1.00 45.79	N
			47.047 28.979 85.323 1.00 46.24	C
ATOM	6025	C ASN D 348	45.907 28.023 85.019 1.00 45.11	С
<b>ATOM</b>	6026	O ASN D 348	45.584 27.686 83.891 1.00 46.36	0
<b>ATOM</b>	6027	CB ASN D 348	48.233 28.214 85.903 1.00 49.70	С
ATOM	6028	CG ASN D 348	48.707 27.068 85.007 1.00 53.34	С
ATOM	6029	OD1 ASN D 348	48.323 25.881 85.136 1.00 54.22	0
<b>ATOM</b>	6030	ND2 ASN D 348	49.568 27.482 84.068 1.00 54.27	N
ATOM	6031	N LEU D 349	45.231 27.538 86.040 1.00 43.17	N
<b>ATOM</b>	6032	CA LEU D 349	44.129 26.598 85.875 1.00 41.36	С
ATOM	6033	C LEU D 349	43.062 27.234 85.022 1.00 41.05	C
		O LEU D 349		0.
		CB LEU D 349		С
			42.504 25.188 87.265 1.00 41.73	С
			42.911 23.883 86.597 1.00 42.98	С
		CD2 LEU D 349		С
		N ALA D 350		N
		CA ALA D 350		С
			42.117 29.313 83.060 1.00 40.66	С
			41.367 28.953 82.161 1.00 39.77	0
ATOM		CB ALA D 350	41.615 30.689 85.022 1.00 39.66	С
		N ASP D 351	43.347 29.758 82.819 1.00 41.67	N
		CA ASP D 351	43.826 29.852 81.455 1.00 43.72	. <b>C</b>
		C ASP D 351	43.624 28.553 80.702 1.00 44.04	С
		O ASP D 351	43.309 28.530 79.516 1.00 44.68	0
		CB ASP D 351	45.277 30.315 81.445 1.00 46.16	C
		CG ASP D 351	45.749 30.472 80.006 1.00 49.30	C
		OD1 ASP D 351	45.392 31.418 79.275 1.00 50.41	0
		OD2 ASP D 351	46,520 29,592 79,570 1.00 51.19	0
		N ARG D 352	43.819 27.406 81.324 1.00 44.03	N
		CA ARG D 352	43.670 26.124 80.674 1.00 44.01	C
		C ARG D 352	42.236 25.737 80.426 1.00 44.62	C
ATOM	6055	O ARG D 352	41.877 25.232 79.361 1.00 44.95	0

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ATOM	6056 CB ARG D 352	44.393 25.123 81.542 1.00 44.71	С
ATOM	6057 CG ARG D 352	45.899 25.219 81.311 1.00 45.89 46.400 23.761 81.449 1.00 47.71	С
ATOM	6058 CD ARG D 352	46.400 23.761 81.449 1.00 47.71	С
ATOM	6059 NE ARG D 352	46.531 23.597 82.889 1.00 50.31	N
ATOM	6060 CZ ARG D 352	46.114 22.564 83.619 1.00 50.39	С
ATOM	6061 NH1 ARG D 352	45.535 21.583 82.950 1.00 49.57	N
ATOM	6062 NH2 ARG D 352	46.380 22.717 84.914 1.00 50.10	N
	6063 N GLUD 353		
		39.923 25.680 81.195 1.00 43.30	
		39.313 26.527 80.081 1.00 43.03	C 0
		38.349 26.140 79.421 1.00 43.08 39.159 25.986 82.467 1.00 42.61	
		39.784 25.428 83.731 1.00 43.36	
ATOM	6069 CD GLUD 353	38.795 25.481 84.878 1.00 43.75	Č
		37.708 24.897 84.813 1.00 43.47	
		39.087 26.148 85.880 1.00 45.48	
		39.872 27.713 79.843 1.00 42.10	N
		39.372 28.627 78.849 1.00 41.53	С
		39.414 27.990 77.488 1.00 41.63	С
		38.515 28.146 76.668 1.00 41.52	
<b>ATOM</b>	6076 CB LEU D 354	40.124 29.967 78.893 1.00 41.46	
		39.490 30.887 79.963 1.00 40.08	С
		40.509 31.876 80.452 1.00 39.39	
		38.254 31.514 79.349 1.00 39.73	
		40.476 27.242 77.253 1.00 42.96	
		40.602 26.533 75.952 1.00 43.04	C
		39.447 25.551 75.825 1.00 43.28	
		38.664 25.632 74.882 1.00 43.52 41.952 25.809 75.905 1.00 40.76	
ATOM	6085 CG1 VAL D 355	42.078 24.985 74.684 1.00 40.75	C
ATOM	6086 CG2 VAL D 355	42.987 26.919 75.932 1.00 42.11	Č
	6087 N HIS D 356	39.302 24.678 76.814 1.00 42.64	N
	6088 CA HIS D 356	38.199 23.750 76.794 1.00 44.51	C
	6089 C HIS D 356	36,873 24,475 76,676 1,00 43,62	С
	6090 O HIS D 356	35.992 24.023 75.945 1.00 42.64	O
<b>ATOM</b>	6091 CB HIS D 356	38.278 22.894 78.084 1.00 48.27	С
ATOM	6092 CG HIS D 356	39.531 22.091 77.914 1.00 51.20	С
	6093 ND1 HIS D 356	39.548 20.794 77.478 1.00 53.46	N
	6094 CD2 HIS D 356	40.812 22.436 78.082 1.00 52.88	C
	6095 CE1 HIS D 356	40.802 20.377 77.407 1.00 53.64	C
	6096 NE2 HIS D 356	41.603 21.351 77.765 1.00 53.38	N
	6097 N MET D 357	36.716 25.583 77.406 1.00 43.17	N
	6098 CA MET D 357	35.488 26.349 77.384 1.00 42.35	C
	6099 C MET D 357	34.999 26.734 75.986 1.00 42.06	C O
ATOM	6100 O MET D 357	33.834 26.548 75.656 1.00 41.73	U

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ΔΤΟΜ	6101 CR MET D 357	35.567 27.657 78.176 1.00 41.83	С
ATOM	6102 CG MET D 357	34.132 28.202 78.315 1.00 40.99	C
ATOM	6103 SD MET D 357	34.234 29.774 79.153 1.00 42.14	S
ATOM	6104 CE MET D 357	34.653 29.240 80.819 1.00 42.38	С
		35.905 27.296 75.206 1.00 40.92	
<b>ATOM</b>	6106 CA ILE D 358	35.618 27.703 73.852 1.00 40.82	С
<b>ATOM</b>	6107 C ILE D 358	35.088 26.509 73.082 1.00 42.56	С
ATOM	6108 O ILE D 358	34.088 26.641 72.391 1.00 43.58	0
ATOM	6109 CB ILE D 358	36.884 28.228 73.142 1.00 39.59	C
		37.398 29.499 73.829 1.00 39.34	
ATOM	6111 CG2 ILE D 358	36.613 28.503 71.697 1.00 37.65	C
ATOM	6112 CD1 ILE D 358	38.667 30.064 73.264 1.00 37.60	C
ATOM	6113 N ASN D 359	35.726 25.354 73.180 1.00 44.35 35.250 24.164 72.492 1.00 46.30	N
ATOM	6114 CA ASN D 359	35.250 24.164 /2.492 1.00 46.30	C C
ATOM	6115 C ASN D 359	33.843 23.838 72.928 1.00 45.64	
ATOM	6110 U ASN D 339	32.962 23.631 72.124 1.00 47.13 36.155 22.978 72.842 1.00 51.34	c
ATOM	6117 CD ASN D 359	37.410 23.123 72.004 1.00 55.99	Ċ
ATOM	6110 ODI ASN D 359	37.180 23.150 70.781 1.00 60.17	Ö
		38.629 23.238 72.519 1.00 57.16	N
ATOM	6121 N TRP D 360	33.592 23.787 74.225 1.00 44.26	
ATOM	6122 CA TRP D 360	32.296 23.479 74.769 1.00 41.88	С
	6123 C TRP D 360		С
ATOM	6124 O TRP D 360	30.110 24.054 73.906 1.00 40.64	0
<b>ATOM</b>	6125 CB TRP D 360	32.435 23.694 76.275 1.00 41.45	С
<b>ATOM</b>	6126 CG TRP D 360	31.082 23.808 76.915 1.00 41.81	С
ATOM	6127 CD1 TRP D 360	30.221 22.791 77.184 1.00 41.25	C
ATOM	6128 CD2 TRP D 360	30.441 25.022 77.348 1.00 41.31	C
ATOM	6129 NEI TRP D 360	29.095 23.305 77.750 1.00 41.05	N
ATOM	6130 CE2 TRP D 360	29.093 23.303 77.730 1.00 41.03 29.198 24.657 77.871 1.00 40.99 30.812 26.369 77.330 1.00 40.72	C C
ATOM	6131 CE3 TRP D 360	28.311 25.581 78.398 1.00 41.54	C
	6132 CZ2 TRP D 360 6133 CZ3 TRP D 360		C
	6134 CH2 TRP D 360		Č
	6135 N ALA D 361	31.562 25.689 74.162 1.00 43.48	N
	6136 CA ALA D 361	30.634 26.720 73.713 1.00 43.83	С
	6137 C ALA D 361	30.132 26.330 72.341 1.00 45.28	С
	6138 O ALA D 361	28.942 26.476 72.114 1.00 46.11	0
ATOM	6139 CB ALA D 361	31.264 28.101 73.696 1.00 42.45	C
	6140 N LYS D 362	30,980 25.849 71.446 1.00 46.93	N
	6141 CA LYS D 362	30.618 25.471 70.112 1.00 48.98	C
	6142 C LYS D 362	29.581 24.390 70.069 1.00 50.09	C
	6143 O LYS D 362	28.874 24.303 69.074 1.00 52.06	0
	6144 CB LYS D 362	31.864 25.075 69.323 1.00 51.99	C
ATOM	6145 CG LYS D 362	32.778 26.268 69.066 1.00 56.03	С

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ΔΤΟΜ	6146 CD LYS D 362	32.135 27.218 68.051 1.00 60.32	С
ATOM	6147 CE LYS D 362	33.091 27.700 66.948 1.00 62.47	C
		32.412 28.297 65.742 1.00 62.21	
ATOM	6149 N ARG D 363	29.375 23.554 71.047 1.00 51.12	N
		28.374 22.527 71.110 1.00 52.21	
	6151 C ARG D 363		C
ATOM	6152 O ARG D 363	26.246 22.058 71.973 1.00 51.12	0
ATOM	6153 CB ARG D 363	28.935 21.320 71.868 1.00 56.54	C C
ATOM	6154 CG ARG D 363	30.449 21.450 71.987 1.00 62.78	C
ATOM	6155 CD ARG D 363	31.016 20.809 70.713 1.00 68.87	N
ATOM	6150 NE ARG D 363	30.663 19.376 70.831 1.00 74.34 31.277 18.626 71.761 1.00 77.66	
ATOM	6157 CZ ARGD 363	32.203 19.186 72.544 1.00 78.42	N
		30.933 17.335 71.872 1.00 79.28	N
ATOM	6160 N VAL D 364	26.934 24.079 72.396 1.00 48.90	N
		25.685 24.397 73.104 1.00 47.37	
ATOM	6162 C VAL D 364	24.686 24.663 72.004 1.00 46.99	С
		24.855 25.578 71.218 1.00 47.63	0
<b>ATOM</b>	6164 CB VAL D 364	25.869 25.635 74.003 1.00 45.65	С
ATOM	6165 CG1 VAL D 364	24.562 26.184 74.492 1.00 44.21	C
		26.780 25.277 75.152 1.00 46.04	
		23.659 23.876 71.871 1.00 47.02	N
		22.645 24.048 70.834 1.00 47.31	С
	6169 C PROD 365		C O
	6170 O PRO D 365		
ATOM	6171 CB PRO D 365	21.458 23.181 71.282 1.00 46.59 22.261 22.071 71.950 1.00 47.00	
ATOM	6173 CD PROD 365	23.391 22.717 72.730 1.00 46.75	
ATOM	6174 N GLY D 366	22.317 26.019 69.422 1.00 47.41	
ATOM	6175 CA GLY D 366	21.964 27.385 69.106 1.00 46.04	С
	6176 C GLY D 366	23.122 28.343 69.012 1.00 45.85	С
		23.086 29.339 68.291 1.00 46.68	0
ATOM		24.190 28.083 69.738 1.00 45.21	N
		25.366 28.929 69.788 1.00 45.52	С
	6180 C PHE D 367	25.976 29.319 68.453 1.00 45.11	C
	6181 O PHE D 367	26.221 30.434 68.001 1.00 43.49	0
	6182 CB PHE D 367	26.477 28.279 70.656 1.00 44.32	C
	6183 CG PHE D 367	27.551 29.268 70.999 1.00 44.55	C C
	6184 CD1 PHE D 367	27.363 30.300 71.898 1.00 44.50	C
		28.773 29.162 70.366 1.00 45.53 28.369 31.197 72.186 1.00 45.11	č
		29.789 30.061 70.658 1.00 46.26	Č
	6188 CZ PHE D 367	29.604 31.087 71.571 1.00 45.31	č
	6189 N VAL D 368	26,265 28.243 67.744 1.00 46.20	N
	6190 CA VAL D 368		C

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ATOM	6101	C VAI D 368	26.082 28.975 65.399 1.00 48.08	С
			26.683 29.387 64.414 1.00 49.17	Ö
			27.205 26.794 66.072 1.00 44.95	C
			26.824 26.469 64.664 1.00 45.34	С
		CG2 VAL D 368		
		N ASP D 369		
			23.954 29.913 64.698 1.00 48.81	С
ATOM	6198	C ASP D 369	24,220 31.395 64.840 1.00 46.53	С
ATOM	6199	O ASP D 369	23.595 32.145 64.116 1.00 47.73 22.469 29.720 65.013 1.00 52.83	0
ATOM	6200	CB ASP D 369	22.469 29.720 65.013 1.00 52.83	С
<b>ATOM</b>	6201	CG ASP D 369	22.039 28.271 64.957 1.00 57.29	С
ATOM	6202	OD1 ASP D 369	22.549 27.486 64.111 1.00 59.44	0
ATOM	6203	OD2 ASP D 369	21.160 27.927 65.791 1.00 59.35	0
ATOM	6204	N LEU D 370	25.002 31.928 65.736 1.00 45.83	N
			25.214 33.375 65.852 1.00 44.35	
			26.392 33.803 65.001 1.00 43.01	
			27.198 32.950 64.652 1.00 43.42	
			25.482 33.706 67.325 1.00 44.43	C
			24.324 33.418 68.273 1.00 44.60	C
			24.659 33.719 69.717 1.00 45.19	
			23.174 34.327 67.868 1.00 45.07	
			26.573 35.055 64.634 1.00 41.97	
			27.740 35.393 63.833 1.00 41.89 28.996 35.122 64.629 1.00 42.57	
			29.066 35.192 65.842 1.00 42.44	
ATOM	6215	CP THR D 371	27.753 36.867 63.472 1.00 42.11	C
ATOM	6217	OGI THR D 371	27.590 37.524 64.730 1.00 44.12	o
			26.588 37.224 62.583 1.00 42.85	
			30.084 34.819 63.921 1.00 44.42	
ATOM	6220	CA LEU D 372	31.352 34.525 64.582 1.00 44.22	С
		C LEU D 372	31.684 35.588 65.615 1.00 45.55	С
		O LEU D 372	32.135 35.219 66.713 1.00 46.54	<b>O</b>
		CB LEU D 372	32.400 34.370 63.500 1.00 43.22	С
		CG LEU D 372	32.274 33.164 62.587 1.00 42.31	С
<b>ATOM</b>	6225	CD1 LEU D 372	33.405 33.206 61.575 1.00 42.37	C.
ATOM	6226	CD2 LEU D 372	32.422 31.864 63.359 1.00 43.20	С
		N HIS D 373	31.476 36.879 65.357 1.00 45.87	N
		CA HIS D 373	31.821 37.871 66.364 1.00 46.42	<b>C</b> .
		C HIS D 373	30.894 37.785 67.553 1.00 45.97	C
		O HIS D 373	31.376 37.912 68.685 1.00 45.63	0
		CB HIS D 373	31,928 39,239 65,738 1.00 48.92	C
		CG HIS D 373	33.222 39.415 64.998 1.00 52.20	C
		ND1 HIS D 373	33.327 39.410 63.612 1.00 54.08	N
		CD2 HIS D 373	34.483 39.619 65.412 1.00 52.17	C
ATOM	6235	CE1 HIS D 373	34.585 39.608 63.254 1.00 53.36	С

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ATOM	6281	CG LEU D 378	26.947 35.482 73.233 1.00 40.01	С
<b>ATOM</b>	6282	CD1 LEU D 378	25.938 34.407 72.906 1.00 39.46	С
<b>ATOM</b>	6283	CD2 LEU D 378	26.289 36.641 73.989 1.00 40.25	С
<b>ATOM</b>		N LEU D 379	31.256 34.725 74.740 1.00 39.51	N
		CA LEU D 379	32.366 34.132 75.452 1.00 38.70	С
		C LEU D 379	33.070 35.171 76.293 1.00 38.95	С
ATOM		O LEU D 379	33.112 35.019 77.509 1.00 37.69	0
ATOM		CB LEUD 379	33.333 33.515 74.462 1.00 38.77	C
ATOM		CG LEUD 379		C
ATOM		_	33.914 31.556 73.159 1.00 40.30	C
ATOM		<del>-</del> ·	33.061 31.264 75.581 1.00 37.03	С
ATOM		N GLUD 380	33.544 36.240 75.642 1.00 40.00	N
		CA GLUD 380		С
		C GLU D 380	33.284 37.785 77.545 1.00 43.10	C
		O GLU D 380	33.718 38.049 78.653 1.00 43.41	0
		CB GLUD 380	34.498 38.490 75.530 1.00 40.94	C
			35.532 38.158 74.456 1.00 43.88	С
		CD GLUD 380		C
		_	34.609 40.105 73.396 1.00 48.71	0
ATOM		OE2 GLU D 380	36.732 39.604 73.006 1.00 47.01	0
ATOM		N CYS D 381	31.981 37.920 77.295 1.00 44.81	N
			31.112 38.377 78.341 1.00 46.63	С
		C CYS D 381		С
		O CYS D 381	31.118 37.898 80.604 1.00 42.78	0
ATOM		CB CYS D 381	29.761 38.864 77.771 1.00 50.78	C
ATOM			29.626 40.658 78.224 1.00 63.43	S
		N ALA D 382	30.743 36.138 79.292 1.00 41.65	N
ATOM		CA ALAD 382	30.518 35.213 80.385 1.00 40.09	C C
ATOM		C ALA D 382	31.613 34.307 80.877 1.00 39.58	0
		O ALA D 382	31.352 33.505 81.778 1.00 39.62	C
ATOM		CB ALAD 382	29.399 34.303 79.819 1.00 38.89	N
		N TRP D 383	32.834 34.376 80.378 1.00 39.40 33.896 33.455 80.771 1.00 38.01	C
		CA TRP D 383	34.029 33.173 82.253 1.00 37.84	C
		C TRP D 383	33.935 32.027 82.709 1.00 36.52	O ·
		O TRP D 383	35.185 33.887 80.105 1.00 36.76	C
		CB TRP D 383 CG TRP D 383	35.874 35.059 80.689 1.00 35.63	C
		CD1 TRP D 383	35.744 36.370 80.365 1.00 35.20	C
			36.869 34.994 81.718 1.00 35.85	c
		CD2 TRP D 383 NE1 TRP D 383	36.573 37.127 81.145 1.00 33.83	N
		CE2 TRP D 383	37.275 36.306 81.987 1.00 34.93	C
		CE2 TRP D 383	37.415 33.946 82.467 1.00 35.33	C
		CZ2 TRP D 383	38,222 36.578 82.953 1.00 35.70	C
		CZ2 TRP D 383	38,348 34,254 83,432 1.00 35.86	C
		CH2 TRP D 383	38.756 35.549 83.663 1.00 35.16	C
ATUM	0323	CU7 1KL D 393	1.00 בטט.נס פאנ.נב טכו	C

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ATOM	6326 N LEUD 384	34.204 34.232 83.045 1.00 37.07	N
ATOM	6327 CA LEU D 384	34.361 34.073 84.485 1.00 34.29	С
ATOM	6328 C LEU D 384	33.083 33.572 85.091 1.00 34.07	С
	6329 O LEUD 384		0
<b>ATOM</b>	6330 CB LEU D 384	34.950 35.349 85.060 1.00 33.01	С
ATOM	6331 CG LEU D 384	35.310 35.329 86.535 1.00 34.01	C
ATOM	6332 CD1 LEU D 384	36.154 34.136 86.972 1.00 34.20	С
		36.009 36.630 86.889 1.00 33.55	С
ATOM	6334 N GLUD 385	31.886 33.919 84.644 1.00 35.06	
		30.648 33.411 85.242 1.00 34.10	C
	6336 C GLUD 385		
	6337 O GLUD 385		0
ATOM	6338 CB GLU D 385	29,414 34.058 84.678 1.00 34.46	C
		28.899 35.317 85.300 1.00 36.30	C C
ATOM	6340 CD GLUD 385	27.712 35.900 84.551 1.00 39.20 27.989 36.563 83.508 1.00 38.66	0
ATOM	6341 OE1 GLU D 383	26.516 35.719 84.973 1.00 40.99	0
		30.940 31.453 83.816 1.00 34.27	N
		31.023 30.042 83.501 1.00 34.27	C
	6345 C ILE D 386		c
ATOM	6346 O T.E.D.386	31.753 28.302 84.965 1.00 36.26	Ö
		31.462 29.651 82.087 1.00 36.16	C
ATOM	6348 CG1 ILE D 386	30.810 30.376 80.921 1.00 38.67	C
ATOM	6349 CG2 ILE D 386	31.205 28.173 81.927 1.00 35.09	С
ATOM	6350 CD1 ILE D 386	29.305 30.310 80.872 1.00 40.67	<b>C</b> .
<b>ATOM</b>	6351 N LEUD 387	33.274 29.877 84.553 1.00 37.57	N
		34.268 29.247 85.404 1.00 36.90	
ATOM	6353 C LEUD 387	33.732 29.174 86.831 1.00 38.44	
		33.820 28.105 87.468 1.00 40.27	0
		35.591 29.959 85.496 1.00 36.96	C
		36,524 29.891 84.290 1.00 38.44	С
	6357 CD1 LEU D 387		С
	6358 CD2 LEU D 387		C
	6359 N MET D 388	33.149 30.263 87.336 1.00 37.63	N
	6360 CA MET D 388		C C
	6361 C MET D 388 6362 O MET D 388	31.539 29.252 88.906 1.00 38.19 31.511 28.579 89.929 1.00 38.89	0
	6363 CB MET D 388	32.289 31.562 89.280 1.00 37.31	C
	6364 CG MET D 388		Č
	6365 SD MET D 388	32.935 34.095 90.117 1.00 39.57	S
	6366 CE MET D 388	34.516 34.928 90.147 1.00 40.10	Č
	6367 N ILE D 389	30.574 29.104 88.001 1.00 40.64	N
	6368 CA ILE D 389	29.485 28.137 88.321 1.00 40.84	C
	6369 C ILE D 389	30.064 26.730 88.304 1.00 41.99	C
	6370 O ILE D 389	29.640 25.844 89.053 1.00 43.43	0
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АТОМ	6371 CB ILE D 389	28.247 28.326 87.427 1.00 37.94	С
ATOM	6372 CG1 ILE D 389	27.068 27.488 87.908 1.00 36.69	C
ATOM	6373 CG2 ILE D 389	28.622 27.941 86.030 1.00 36.39	C
ATOM	6374 CD1 ILE D 389	25.732 27.888 87.384 1.00 34.40	С
		31.076 26.487 87.474 1.00 41.93	
ATOM	6376 CA GLY D 390	31.680 25.159 87.421 1.00 42.20	С
		32.294 24.860 88.770 1.00 42.14	
ATOM	6378 O GLY D 390	32.038 23.806 89.321 1.00 41.64	0
<b>ATOM</b>	6379 N LEU D 391	33.068 25.848 89.246 1.00 42.56 33.741 25.678 90.541 1.00 41.55	N
<b>ATOM</b>	6380 CA LEU D 391	33.741 25.678 90.541 1.00 41.55	С
<b>ATOM</b>	6381 C LEU D 391	32.731 25.332 91.599 1.00 41.30	С
ATOM	6382 O LEU D 391	32.765 24.333 92.268 1.00 42.41	O
<b>ATOM</b>	6383 CB LEUD 391	34.471 26.946 90.967 1.00 40.77	С
ATOM	6384 CG LEU D 391	35.090 27.007 92.349 1.00 41.23	C
ATOM	6385 CD1 LEU D 391	36.095 25.868 92.543 1.00 41.69	С
		35.784 28.323 92.643 1.00 41.15	
ATOM	6387 N VAL D 392	31.757 26.194 91.775 1.00 42.54	N
ATOM	6388 CA VAL D 392	30.712 26.047 92.770 1.00 42.50	C
		30.087 24.673 92.725 1.00 44.06	
		29.878 24.012 93.738 1.00 44.87	
ATOM	6391 CB VAL D 392	29.661 27.150 92.609 1.00 41.04	C
ATOM	6392 CG1 VAL D 392	28.457 26.838 93.465 1.00 40.61	C C
		30.233 28.468 93.091 1.00 40.68	
		29.749 24.233 91.530 1.00 45.63	
ATOM	6393 CA TRP D 393	29.106 22.954 91.287 1.00 46.45	
ATOM	6390 C TRP D 393	29.993 21.800 91.697 1.00 46.87 29.499 20.900 92.357 1.00 47.71	o
ATOM	6309 CB TBB D 303	28.821 22.832 89.788 1.00 47.71	Č
		28.626 21.413 89.360 1.00 47.45	
ATOM	6400 CD1 TRP D 393	29 474 20 649 88 625 1 00 47 21	
ATOM	6401 CD2 TRP D 393	29.474 20.649 88.625 1.00 47.21 27.495 20.592 89.658 1.00 47.89	Č
	6402 NE1 TRP D 393	28.934 19.407 88.437 1.00 47.18	N
	6403 CE2 TRP D 393	27.722 19.336 89.057 1.00 47.38	C
	6404 CE3 TRP D 393	26,314 20.800 90.373 1.00 48.23	С
	6405 CZ2 TRP D 393	26.821 18.281 89.148 1.00 47.14	C
	6406 CZ3 TRP D 393	25.423 19.753 90.471 1.00 48.58	С
<b>ATOM</b>	6407 CH2 TRP D 393	25.683 18.514 89.859 1.00 48.15	С
<b>ATOM</b>	6408 N ARG D 394	31.261 21.843 91.276 1.00 47.26	N
<b>ATOM</b>	6409 CA ARG D 394	32.153 20.755 91.647 1.00 47.47	C
<b>ATOM</b>	6410 C ARG D 394	32.522 20.880 93.110 1.00 48.85	С
	6411 O ARG D 394	32.965 19.910 93.710 1.00 51.34	0
	6412 CB ARG D 394	33.346 20.565 90.751 1.00 45.88	С
	6413 CG ARG D 394	34.195 21.670 90.285 1.00 45.23	C
	6414 CD ARG D 394		С
ATOM	6415 NE ARG D 394	36.333 22.366 89.420 1.00 44.88	N

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		34.787 24.865 102.689 1.00 56.74	C O
		35.733 25.606 103.049 1.00 57.61	_
		34.827 24.116 101.596 1.00 55.26	N C
		35.988 24.084 100.747 1.00 55.15	C
	6465 C LYS D 401		
		34.456 24.152 98.883 1.00 53.30	O C
		36.607 22.703 100.773 1.00 57.46	C
ATOM	6468 CG LYSD 401	36.857 22.055 102.095 1.00 60.83 38.357 21.996 102.346 1.00 64.64	C
			C
		38.622 21.658 103.805 1.00 67.58	
		37.772 20.479 104.196 1.00 70.44	N
ATOM	6472 N LEU D 402	36.677 24.687 98.529 1.00 51.63	N
		36.481 24.885 97.108 1.00 49.28	С
		37.432 23.955 96.365 1.00 48.72	C
ATOM	6475 O LEU D 402	38.646 24.038 96.510 1.00 49.51	0
ATOM	6476 CB LEU D 402	36.691 26.311 96.652 1.00 48.95 35.857 27.437 97.251 1.00 48.74	С
ATOM	6477 CG LEU D 402	35,857 27,437 97,251 1.00 48.74	C
		36.524 28.796 97.010 1.00 48.73	C C
		34.438 27.390 96.713 1.00 47.64	
		36.886 23.079 95.559 1.00 47.56	N C
		37.661 22.157 94.763 1.00 47.51	C
		38.046 22.737 93.418 1.00 47.68	0
		37.391 22.436 92.405 1.00 48.52	C
ATOM	6484 CB LEU D 403	36.733 20.948 94.527 1.00 48.78	C
ATOM	6485 CG LEU D 403	37.468 19.675 94.109 1.00 49.22	C
		37.960 18.999 95.365 1.00 49.67	C
		36.624 18.756 93.259 1.00 48.96	N
	6488 N PHE D 404	39.100 23.533 93.300 1.00 46.77	C
	6489 CA PHE D 404	39.468 24.057 91.990 1.00 46.19	c
ATOM		39.733 22.892 91.068 1.00 47.69	0
		39.366 22.906 89.903 1.00 48.97	C
	6492 CB PHE D 404		. C .
	6493 CG PHE D 404	40.214 26.288 92.661 1.00 45.16 40.200 26.430 94.033 1.00 44.79	C
	6494 CD1 PHE D 404	39.788 27.331 91.850 1.00 45.19	C.
	6495 CD2 PHE D 404	39.754 27.624 94.587 1.00 45.59	C
	6496 CE1 PHE D 404	39.734 27.624 94.387 1.00 43.39	C
		39.349 28.321 92.383 1.00 44.20 39.339 28.659 93.752 1.00 45.30	Č
	6498 CZ PHE D 404 6499 N ALA D 405	40.410 21.876 91.548 1.00 50.13	N
		40.730 20.666 90.804 1.00 52.20	C
	6500 CA ALA D 405 6501 C ALA D 405	40.730 20.666 90.804 1.00 32.20	c
	6502 O ALA D 405	40.430 19.522 92.927 1.00 54.84	Ö
	6503 CB ALA D 405	42.170 20.689 90.327 1.00 51.92	C
		40.555 18.288 91.120 1.00 53.68	N
	6505 CA PRO D 406	40.455 17.023 91.830 1.00 53.61	C
ATUM	0303 CA PROD 400	17.02 71.02 1.00 JJ.01	C

ATOM 6506 C PRO D 406 ATOM 6507 O PRO D 406 ATOM 6508 CB PRO D 406 ATOM 6509 CG PRO D 406 ATOM 6510 CD PRO D 406 ATOM 6510 CD PRO D 406 ATOM 6511 N ASN D 407 ATOM 6512 CA ASN D 407 ATOM 6513 C ASN D 407 ATOM 6515 CB ASN D 407 ATOM 6516 CG ASN D 407 ATOM 6516 CG ASN D 407 ATOM 6516 CG ASN D 407 ATOM 6517 OD1 ASN D 407 ATOM 6518 ND2 ASN D 407 ATOM 6519 N LEUD 408 ATOM 6520 CA LEUD 408 ATOM 6521 C LEUD D 408 ATOM 6522 O LEUD 408 ATOM 6523 CB LEUD 408 ATOM 6525 CDI LEUD 408 ATOM 6526 CD2 LEUD 408 ATOM 6526 CD2 LEUD 409 ATOM 6537 N LEUD 409 ATOM 6530 O LEUD 409 ATOM 6531 CB LEUD 409 ATOM 6531 CB LEUD 409 ATOM 6532 CG LEUD 409 ATOM 6533 CG LEUD 409 ATOM 6534 CD2 LEUD 409 ATOM 6537 C LEUD 410 ATOM 6538 CA LEUD 410 ATOM 6538 CA LEUD 410 ATOM 6539 CB LEUD 410 ATOM 6539 CB LEUD 410 ATOM 6530 CB LEUD 410 ATOM 6531 CB LEUD 410 ATOM 6532 CG LEUD 410 ATOM 6534 CD2 LEUD 410 ATOM 6536 CA LEUD 410 ATOM 6537 C LEUD 410 ATOM 6538 CA LEUD 410 ATOM 6538 CA LEUD 410 ATOM 6540 CG LEUD 410 ATOM 6541 CD1 LEUD 410 ATOM 6541 CD2 LEUD 410 ATOM 6542 CD2 LEUD 410 ATOM 6544 CA ASP D 411 ATOM 6545 C ASP D 411 ATOM 6546 CA ASP D 411 ATOM 6547 CB ASP D 411 ATOM 6548 CG ASP D 411 ATOM 6559 OD2 ASP D 411 ATOM 6550 OD2 ASP D 411	wo	98/56812	254/371	PCT/GB98/01708
ATOM 6507 O PRO D 406 ATOM 6508 CB PRO D 406 ATOM 6509 CG PRO D 406 ATOM 6510 CD PRO D 406 ATOM 6511 N ASND 407 ATOM 6512 CA ASND 407 ATOM 6513 C ASND 407 ATOM 6514 O ASND 407 ATOM 6516 CG ASND 407 ATOM 6516 CG ASND 407 ATOM 6516 CG ASND 407 ATOM 6517 ODI ASND 407 ATOM 6518 ND2 ASND 407 ATOM 6518 ND2 ASND 407 ATOM 6519 N LEUD 408 ATOM 6520 CA LEUD 408 ATOM 6521 C LEUD 408 ATOM 6521 C LEUD 408 ATOM 6522 CD LEUD 408 ATOM 6523 CB LEUD 408 ATOM 6524 CG LEUD 408 ATOM 6525 CD1 LEUD 408 ATOM 6526 CD2 LEUD 408 ATOM 6527 N LEUD 409 ATOM 6531 CB LEUD 409 ATOM 6532 CD LEUD 409 ATOM 6534 CD 2 LEUD 409 ATOM 6536 CA LEUD 409 ATOM 6537 C LEUD 410 ATOM 6538 CD LEUD 410 ATOM 6538 CD LEUD 410 ATOM 6544 CG ASP D 411 ATOM 6546 CA ASP D 411 ATOM 6547 CB ASP D 411 ATOM 6549 ODI ASP D 411 ATOM 6549 ODI ASP D 411 ATOM 6549 ODI ASP D 411 ATOM 6540 CA ASP D 411 ATOM 6540 CA ASP	АТОМ	6506 C PRO D 406		С
ATOM 6508 CB PRO D 406 ATOM 6509 CG PRO D 406 ATOM 6510 CD PRO D 406 ATOM 6510 CD PRO D 406 ATOM 6511 N ASN D 407 ATOM 6512 CA ASN D 407 ATOM 6513 C ASN D 407 ATOM 6514 O ASN D 407 ATOM 6515 CB ASN D 407 ATOM 6515 CB ASN D 407 ATOM 6516 CG ASN D 407 ATOM 6517 OD1 ASN D 407 ATOM 6518 ND2 ASN D 407 ATOM 6518 ND2 ASN D 407 ATOM 6519 N LEUD 408 ATOM 6520 CA LEUD 408 ATOM 6521 C LEUD 408 ATOM 6521 C LEUD 408 ATOM 6522 CG LEUD 408 ATOM 6525 CD1 LEUD 408 ATOM 6526 CD2 LEUD 408 ATOM 6526 CD2 LEUD 409 ATOM 6530 O LEUD 409 ATOM 6531 CB LEUD 409 ATOM 6531 C B ASN D 407 ATOM 6531 C S ASN D 407 ATOM 6531 CB LEUD 408 ATOM 6526 CD2 LEUD 408 ATOM 6527 N LEUD 408 ATOM 6528 CA LEUD 409 ATOM 6530 O LEUD 409 ATOM 6531 CB LEUD 409 ATOM 6531 CB LEUD 409 ATOM 6531 CB LEUD 409 ATOM 6532 CG LEUD 409 ATOM 6531 CB LEUD 409 ATOM 6534 CD2 LEUD 409 ATOM 6534 CD2 LEUD 409 ATOM 6536 CA LEUD 409 ATOM 6536 CA LEUD 409 ATOM 6537 C LEUD 409 ATOM 6538 O LEUD 410 ATOM 6536 CA LEUD 410 ATOM 6537 C LEUD 410 ATOM 6536 CA LEUD 410 ATOM 6536 CA LEUD 410 ATOM 6537 C LEUD 410 ATOM 6536 CA LEUD 410 ATOM 6536 CA LEUD 410 ATOM 6537 C LEUD 410 ATOM 6538 O LEUD 410 ATOM 6536 CA LEUD 410 ATOM 6537 C LEUD 410 ATOM 6538 C ALEUD 410 ATOM 6536 CA LEUD 410 ATOM 6537 C LEUD 410 ATOM 6536 CA LEUD 410 ATOM 6536 CA LEUD 410 ATOM 6537 C LEUD 410 ATOM 6538 O LEUD 410 ATOM 6534 CA LEUD 410 ATOM 6534 CD LEUD 410 ATOM 6535 C LEUD 410 ATOM 6540 CA ASP D 411 ATOM 6540 CA ASP D 411 ATOM 6545 C ASP D 411 ATOM 6546 CA ASP D 411 ATOM 6546 CA ASP D 411 ATOM 6547 CB ASP D 411 ATOM 6548 CG ASP D 411 ATOM 6548 CG ASP D 411 ATOM 6549 OD1 ASP D 411 ATOM 6549 OD1 ASP D 411 ATOM 6540 CB ASP D 411 ATOM 6540 CB ASP D 411 ATOM 6540 OD1 ASP D 411 AT	ATOM	6507 O PRO D 406	41 444 16 490 93.860 1.00 56.81	
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ATOM 6541 CD1 LEU D 410				
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ATOM 6548 CG ASP D 411 40.349 25.738 104.655 1.00 71.89 C ATOM 6549 OD1 ASP D 411 40.851 26.870 104.877 1.00 73.52 O				
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ATOM 6550 OD2 ASP D 411 39.629 25.053 105.439 1.00 74.78 O				Ο
	ATOM	6550 OD2 ASP D 411	39.629 25.053 105.439 1.00 74.78	0

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ATOM 6596 CB CYS D 417 ATOM 6597 SG CYS D 417 ATOM 6598 N VAL D 418 ATOM 6599 CA VAL D 418 ATOM 6699 CA VAL D 418 ATOM 6601 C VAL D 418 ATOM 6601 C VAL D 418 ATOM 6602 CB VAL D 418 ATOM 6603 CGI VAL D 418 ATOM 6603 CGI VAL D 418 ATOM 6605 N GLU D 419 ATOM 6606 CA GLU D 419 ATOM 6606 C GB CUD 419 ATOM 6606 C GB CUD 419 ATOM 6606 C GB CUD 419 ATOM 6608 C GB CUD 419 ATOM 6609 CB GLU D 419 ATOM 6609 CB GLU D 419 ATOM 6610 C G GLU D 419 ATOM 6611 CD GLU D 419 ATOM 6612 C GE GLU D 419 ATOM 6614 N GLY D 420 ATOM 6615 C A GLY D 420 ATOM 6616 C GLY D 420 ATOM 6616 C GLY D 420 ATOM 6616 C GLY D 420 ATOM 6617 C GLU D 419 ATOM 6618 N MET D 421 ATOM 6620 C MET D 421 ATOM 6630 CB VAL D 422 ATOM 6631 CGI VAL D 422 ATOM 6634 CA GLU D 423 ATOM 6636 C GLU D 423 ATOM 6	. wo	98/56812	256/371	PCT/GB98/01708
ATOM 6598 N VAL D 418	4 TO 1 4	6506 CD CVS D 417	47 262 32 815 100 634 1 00 68 39	C
ATOM 6598 N VAL D 418	ATOM	6590 CB C15 D 417	47 427 31 592 101 951 1.00 73.49	Š
ATOM 6599 CA VAL D 418 ATOM 6601 C VAL D 418 ATOM 6601 C VAL D 418 ATOM 6601 C VAL D 418 ATOM 6602 CB VAL D 418 ATOM 6603 CGI VAL D 418 ATOM 6603 CGI VAL D 418 ATOM 6604 CG2 VAL D 418 ATOM 6605 N GLUD 419 ATOM 6606 CA GLUD 419 ATOM 6606 CA GLUD 419 ATOM 6607 C GLUD 419 ATOM 6608 O GLUD 419 ATOM 6608 CG GLUD 419 ATOM 6610 CG GLUD 419 ATOM 6611 CD GLUD 419 ATOM 6612 OEI GLUD 419 ATOM 6613 OEZ GLUD 419 ATOM 6614 N GLY D 420 ATOM 6615 CA GLYD 420 ATOM 6616 C GLY D 420 ATOM 6616 C GLY D 420 ATOM 6617 O GLY D 420 ATOM 6618 N MET D 421 ATOM 6620 C MET D 421 ATOM 6620 C MET D 421 ATOM 6621 O MET D 421 ATOM 6622 CB MET D 421 ATOM 6624 SD MET D 421 ATOM 6625 CE MET D 421 ATOM 6625 CE MET D 421 ATOM 6626 N VAL D 422 ATOM 6626 CR VAL D 422 ATOM 6631 CGI VAL D 422 ATOM 6631 CGI VAL D 422 ATOM 6632 CG WET D 421 ATOM 6634 CA GLUD 422 ATOM 6635 C GLUD 423 ATOM 6637 CA VAL D 422 ATOM 6638 CG VAL D 422 ATOM 6630 CG VAL D 422 ATOM 6631 CGI VAL D 422 ATOM 6631 CGI VAL D 422 ATOM 6632 CG VAL D 422 ATOM 6634 CA GLUD 423 ATOM 6635 C GLUD 423 ATOM 6636 C GLUD 423 ATOM 6635 C GLUD 423 ATOM 6636 C GLUD 423 ATO	ATOM	6598 N VAL D 418	45.893 35.461 99.383 1.00 62.39	N
ATOM 6600 C VAL D 418				
ATOM 6601 O VAL D 418 ATOM 6602 CB VAL D 418 ATOM 6603 CG1 VAL D 418 ATOM 6603 CG1 VAL D 418 ATOM 6604 CG2 VAL D 418 ATOM 6605 N GLUD 419 ATOM 6606 CA GLUD 419 ATOM 6606 CA GLUD 419 ATOM 6606 CA GLUD 419 ATOM 6607 C GLUD 419 ATOM 6608 O GLUD 419 ATOM 6609 CB GLUD 419 ATOM 6610 CG GLUD 419 ATOM 6610 CG GLUD 419 ATOM 6610 CG GLUD 419 ATOM 6611 CD GLUD 419 ATOM 6611 CD GLUD 419 ATOM 6612 OE1 GLUD 419 ATOM 6615 CA GLYD 420 ATOM 6615 CA GLYD 420 ATOM 6615 CA GLYD 420 ATOM 6616 C GLYD 420 ATOM 6616 C GLYD 420 ATOM 6617 O GLYD 420 ATOM 6618 N MET D 421 ATOM 6619 CA MET D 421 ATOM 6620 C MET D 421 ATOM 6621 O MET D 421 ATOM 6622 CB MET D 421 ATOM 6623 CG MET D 421 ATOM 6624 SD MET D 421 ATOM 6625 CE MET D 421 ATOM 6626 N VAL D 422 ATOM 6626 CB VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6631 CG CB VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6631 CG VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6631 CG VAL D 422 ATOM 6632 CG VAL D 422 ATOM 6632 CG VAL D 422 ATOM 6634 CA GLUD 423 ATOM 6635 C GLUD 423 ATOM 6635 C GLUD 423 ATOM 6636 C GLUD 423 ATOM 6636 CG GLUD 42	ATOM	6600 C VAL D 418	44,980 37.688 98.902 1.00 61.04	С
ATOM 6602 CB VALD 418 ATOM 6603 CG1 VALD 418 ATOM 6604 CG2 VALD 418 ATOM 6605 N GLUD 419 ATOM 6606 CA GLUD 419 ATOM 6606 CA GLUD 419 ATOM 6607 C GLUD 419 ATOM 6608 O GLUD 419 ATOM 6609 CB GLUD 419 ATOM 6610 CG GLUD 419 ATOM 6610 CG GLUD 419 ATOM 6611 CD GLUD 419 ATOM 6612 OE1 GLUD 419 ATOM 6613 OE2 GLUD 419 ATOM 6616 C GLYD 420 ATOM 6615 CA GLYD 420 ATOM 6616 C GLYD 420 ATOM 6617 O GLYD 420 ATOM 6618 N MET D 421 ATOM 6619 CA MET D 421 ATOM 6620 C MET D 421 ATOM 6620 C MET D 421 ATOM 6622 CB MET D 421 ATOM 6623 CG MET D 421 ATOM 6624 SD MET D 421 ATOM 6625 CE MET D 421 ATOM 6626 CR VALD 422 ATOM 6630 CB VALD 422 ATOM 6630 CB VALD 422 ATOM 6631 CG1 VALD 422 ATOM 6631 CG2 VALD 422 ATOM 6632 CG2 VALD 422 ATOM 6631 CG1 VALD 422 ATOM 6632 CG2 VALD 422 ATOM 6630 CB VALD 422 ATOM 6630 CB VALD 422 ATOM 6631 CG1 VALD 422 ATOM 6631 CG1 VALD 422 ATOM 6632 CG2 VALD 422 ATOM 6634 CA GLUD 423 ATOM 6635 C GLUD 423 ATOM 6636 CG CG VALD 422 ATOM 6630 CB VALD 422 ATOM 6631 CG1 VALD 422 ATOM 6634 CA GLUD 423 ATOM 6635 C GLUD 423 ATOM 6635 C GLUD 423 ATOM 6636 CG	ATOM	6601 O VAL D 418	43.903 37.466 99.445 1.00 60.87	
ATOM 6603 CG1 VAL D 418 ATOM 6604 CG2 VAL D 418 ATOM 6605 N GLU D 419 ATOM 6606 CA GLU D 419 ATOM 6606 CA GLU D 419 ATOM 6607 C GLU D 419 ATOM 6608 O GLU D 419 ATOM 6608 O GLU D 419 ATOM 6609 CB GLU D 419 ATOM 6610 CG GLU D 419 ATOM 6610 CG GLU D 419 ATOM 6611 CD GLU D 419 ATOM 6612 CB GLU D 419 ATOM 6613 OE2 GLU D 419 ATOM 6615 CA GLY D 420 ATOM 6616 C GLY D 420 ATOM 6616 C GLY D 420 ATOM 6616 C GLY D 420 ATOM 6617 O GLY D 420 ATOM 6618 N MET D 421 ATOM 6619 CA MET D 421 ATOM 6620 C MET D 421 ATOM 6620 C MET D 421 ATOM 6621 CB MET D 421 ATOM 6622 CB MET D 421 ATOM 6624 SD MET D 421 ATOM 6625 CE MET D 421 ATOM 6626 N VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6631 CG1 VAL D 422 ATOM 6631 CG1 VAL D 422 ATOM 6631 CG1 VAL D 422 ATOM 6632 CG2 VAL D 422 ATOM 6634 CA GLU D 423 ATOM 6635 C GLU D 423 ATOM 6636 C GLU D 422 ATOM 6636 C GLU D 422 ATOM 6630 CB VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6631 CG1 VAL D 422 ATOM 6634 CA GLU D 423 ATOM 6635 C GLU D 423 ATOM 6635 C GLU D 423 ATOM 6636	ATOM	6602 CB VAL D 418	45.360 36.041 97.073 1.00 59.10	
ATOM 6605 N GLUD 419	ATOM	6603 CG1 VAL D 418	45.183 37.173 96.080 1.00 58.79	
ATOM 6606 CA GLUD 419	ATOM	6604 CG2 VAL D 418	46.314 34.983 96.546 1.00 58.31	
ATOM 6607 C GLUD 419 ATOM 6608 O GLUD 419 ATOM 6608 O GLUD 419 ATOM 6608 O GLUD 419 ATOM 6609 CB GLUD 419 ATOM 6600 CG GLUD 419 ATOM 6610 CG GLUD 419 ATOM 6611 CD GLUD 419 ATOM 6611 CD GLUD 419 ATOM 6612 OE1 GLUD 419 ATOM 6613 OE2 GLUD 419 ATOM 6614 N GLY D 420 ATOM 6616 C GLY D 420 ATOM 6616 C GLY D 420 ATOM 6616 C GLY D 420 ATOM 6617 O GLY D 420 ATOM 6618 N MET D 421 ATOM 6619 CA MET D 421 ATOM 6620 C MET D 421 ATOM 6621 O MET D 421 ATOM 6622 CB MET D 421 ATOM 6623 CG MET D 421 ATOM 6624 SD MET D 421 ATOM 6625 CE MET D 421 ATOM 6626 N VAL D 422 ATOM 6627 CA VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6631 CG GLUD 423 ATOM 6631 CG GLUD 423 ATOM 6634 CA GLUD 423 ATOM 6634 CA GLUD 423 ATOM 6636 O GLUD 423 ATOM 6635 C GLUD 423 ATOM 6636 O GLUD 423 ATOM 6635 C GLUD 423 ATOM 6636 O GLUD 423	ATOM	6605 N GLUD 419	45.428 38.912 98.712 1.00 62.71	· ·
ATOM 6608 O GLU D 419	ATOM	6606 CA GLUD 419	44.716 40.116 99.093 1.00 65.35	
ATOM 6609 CB GLUD 419	ATOM	6607 C GLUD 419	43.332 40.190 98.494 1.00 64.60	
ATOM 6610 CG GLUD 419 ATOM 6611 CD GLUD 419 ATOM 6611 CD GLUD 419 ATOM 6612 OE1 GLUD 419 ATOM 6613 OE2 GLUD 419 ATOM 6614 N GLYD 420 ATOM 6615 CA GLYD 420 ATOM 6616 C GLYD 420 ATOM 6616 C GLYD 420 ATOM 6617 O GLYD 420 ATOM 6618 N MET D 421 ATOM 6618 N MET D 421 ATOM 6620 C MET D 421 ATOM 6621 O MET D 421 ATOM 6620 C MET D 421 ATOM 6620 C MET D 421 ATOM 6621 CG MET D 421 ATOM 6620 C MET D 421 ATOM 6620 C MET D 421 ATOM 6621 CG MET D 421 ATOM 6620 C MET D 421 ATOM 6620 C MET D 421 ATOM 6621 CG MET D 421 ATOM 6620 C MET D 421 ATOM 6620 C MET D 421 ATOM 6621 CG MET D 421 ATOM 6622 CG MET D 421 ATOM 6625 CE MET D 421 ATOM 6626 N VAL D 422 ATOM 6627 CA VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6631 CG1 VAL D 422 ATOM 6631 CG1 VAL D 422 ATOM 6632 CG2 VAL D 422 ATOM 6634 CA GLUD 423 ATOM 6635 C GLUD 423 ATOM 6636 C GLUD 423	ATOM	6608 O GLUD 419	43.065 39.945 97.322 1.00 65.26	
ATOM 6611 CD GLUD 419 ATOM 6612 OE1 GLUD 419 ATOM 6613 OE2 GLUD 419 ATOM 6613 OE2 GLUD 419 ATOM 6614 N GLYD 420 ATOM 6615 CA GLYD 420 ATOM 6616 C GLYD 420 ATOM 6616 C GLYD 420 ATOM 6617 O GLYD 420 ATOM 6618 N MET D 421 ATOM 6619 CA MET D 421 ATOM 6620 C MET D 421 ATOM 6620 C MET D 421 ATOM 6622 CB MET D 421 ATOM 6624 SD MET D 421 ATOM 6625 CE MET D 421 ATOM 6626 N VAL D 422 ATOM 6626 C VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6631 CG CLYD 422 ATOM 6630 C GLYD 422 ATOM 6631 CG CLYD 423 ATOM 6635 C GLUD 423 ATOM 6636 O GLUD 423 ATOM 6637 R98.970 1.00 55.62 ATOM 6636 O GLUD 423 ATOM 6636 O GLUD 423 ATOM 6636 O GLUD 423 ATOM 6637 R98.970 1.00 55.62 C C C C C C C C C C C C C C C C C C C	ATOM	6609 CB GLUD 419	45.537 41.284 98.568 1.00 70.24	
ATOM 6612 OE1 GLU D 419 ATOM 6613 OE2 GLU D 419 ATOM 6614 N GLY D 420 ATOM 6615 CA GLY D 420 ATOM 6616 C GLY D 420 ATOM 6617 O GLY D 420 ATOM 6618 N MET D 421 ATOM 6618 N MET D 421 ATOM 6619 CA MET D 421 ATOM 6620 C MET D 421 ATOM 6621 O MET D 421 ATOM 6622 CB MET D 421 ATOM 6624 SD MET D 421 ATOM 6625 CE MET D 421 ATOM 6626 N VAL D 422 ATOM 6626 N VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6630 CG VAL D 422 ATOM 6630 CG CU D 423 ATOM 6630 CG CJU D 423 ATOM 6631 CG CJU D 423 ATOM 6635 C GLU D 423 ATOM 6636 O GLU D 423 ATOM 6636 O GLU D 423 ATOM 6637 CA CJU D 423 ATOM 6637 CA CJU D 423 ATOM 6638 C CJU D 423 ATOM 6636 O GLU D 423 ATOM 6637 CA CJU D 423 ATOM 6637 CA CJU D 423 ATOM 6638 C CJU D 423 ATOM 6637 CA CJU D 423 ATOM 6637 CA CJU D 423 ATOM 6638 C CJU D 423 ATOM 6637 CA CJU D 423 ATOM 6637 CA CJU D 423 ATOM 6638 C CJU D 423 ATOM 6637 CA CJU D 423 ATOM 6638 CA GLU D 423 ATOM 6637 CA GLU D 423 ATOM 6638 CA GLU D 423 ATOM 6637 CA GLU D 423 ATOM 6638 CA GLU D 423 ATOM 6639 CA GLU D 423 ATOM 6636 O GLU D 423	ATOM	6610 CG GLUD 419	45.008 42.507 99.451 1.00 70.95	
ATOM 6614 N GLY D 420 ATOM 6615 CA GLY D 420 ATOM 6616 C GLY D 420 ATOM 6616 C GLY D 420 ATOM 6617 O GLY D 420 ATOM 6618 N MET D 421 ATOM 6619 CA MET D 421 ATOM 6619 CA MET D 421 ATOM 6620 C MET D 421 ATOM 6620 C MET D 421 ATOM 6620 C MET D 421 ATOM 6620 CB MET D 421 ATOM 6620 CB MET D 421 ATOM 6624 SD MET D 421 ATOM 6625 CE MET D 421 ATOM 6626 N VAL D 422 ATOM 6627 CA VAL D 422 ATOM 6628 C VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6631 CG1 VAL D 422 ATOM 6631 CG1 VAL D 422 ATOM 6631 CG1 VAL D 422 ATOM 6632 CG2 VAL D 422 ATOM 6633 N GLU D 423 ATOM 6634 CA GLU D 423 ATOM 6635 C GLU D 423 ATOM 6635 C GLU D 423 ATOM 6636 O GLU D 423	ATOM	6611 CD GLUD 419	46.113 43.738 98.083 1.00 81.24	0
ATOM 6614 N GLY D 420 ATOM 6615 CA GLY D 420 ATOM 6616 C GLY D 420 ATOM 6616 C GLY D 420 ATOM 6617 O GLY D 420 ATOM 6618 N MET D 421 ATOM 6619 CA MET D 421 ATOM 6619 CA MET D 421 ATOM 6620 C MET D 421 ATOM 6620 C MET D 421 ATOM 6620 C MET D 421 ATOM 6620 CB MET D 421 ATOM 6620 CB MET D 421 ATOM 6624 SD MET D 421 ATOM 6625 CE MET D 421 ATOM 6626 N VAL D 422 ATOM 6627 CA VAL D 422 ATOM 6628 C VAL D 422 ATOM 6630 CB VAL D 422 ATOM 6631 CG1 VAL D 422 ATOM 6631 CG1 VAL D 422 ATOM 6631 CG1 VAL D 422 ATOM 6632 CG2 VAL D 422 ATOM 6633 N GLU D 423 ATOM 6634 CA GLU D 423 ATOM 6635 C GLU D 423 ATOM 6635 C GLU D 423 ATOM 6636 O GLU D 423	ATOM	6612 OE1 GLU D 419	45.606 44.880 00.073 1.00 82.02	0
ATOM 6615 CA GLY D 420	ATOM	6614 N GIVD 419	42 312 40 504 99 261 1 00 64 31	N
ATOM 6616 C GLY D 420	ATOM	6615 CA GI Y D 420	40 952 40 618 98 782 1 00 63.52	
ATOM 6617 O GLY D 420 39.132 39.494 97.866 1.00 63.85 O ATOM 6618 N MET D 421 40.830 38.189 98.353 1.00 61.96 N ATOM 6619 CA MET D 421 40.233 36.958 97.909 1.00 61.23 C ATOM 6620 C MET D 421 39.229 36.266 98.798 1.00 60.15 C ATOM 6621 O MET D 421 38.393 35.534 98.295 1.00 60.63 O ATOM 6622 CB MET D 421 41.368 35.916 97.784 1.00 62.22 C ATOM 6623 CG MET D 421 41.916 35.960 96.369 1.00 63.61 C ATOM 6624 SD MET D 421 41.148 34.624 95.448 1.00 63.00 S ATOM 6625 CE MET D 421 42.379 33.382 95.900 1.00 65.22 C ATOM 6626 N VAL D 422 39.313 36.410 100.099 1.00 59.43 N ATOM 6627 CA VAL D 422 38.441 35.785 101.056 1.00 58.24 C ATOM 6629 O VAL D 422 36.983 36.109 100.795 1.00 57.82 C ATOM 6630 CB VAL D 422 38.661 36.226 102.514 1.00 58.54 C ATOM 6631 CG1 VAL D 422 38.861 36.226 102.514 1.00 58.54 C ATOM 6632 CG2 VAL D 422 38.8661 36.226 102.514 1.00 59.06 C ATOM 6634 CA GLU D 423 36.646 37.343 100.455 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46	ATOM	6616 C GLY D 420	40 278 39 372 98 291 1.00 62.66	
ATOM 6618 N MET D 421				
ATOM 6619 CA MET D 421	ATOM	6618 N MET D 421	40,830 38,189 98,353 1.00 61.96	N
ATOM 6620 C MET D 421 39.229 36.266 98.798 1.00 60.15 C ATOM 6621 O MET D 421 38.393 35.534 98.295 1.00 60.63 O ATOM 6622 CB MET D 421 41.368 35.916 97.784 1.00 62.22 C ATOM 6623 CG MET D 421 41.916 35.960 96.369 1.00 63.61 C ATOM 6624 SD MET D 421 41.148 34.624 95.448 1.00 63.00 S ATOM 6625 CE MET D 421 42.379 33.382 95.900 1.00 65.22 C ATOM 6626 N VAL D 422 39.313 36.410 100.099 1.00 59.43 N ATOM 6627 CA VAL D 422 36.983 36.109 100.795 1.00 57.82 C ATOM 6628 C VAL D 422 36.983 36.109 100.795 1.00 57.82 C ATOM 6630 CB VAL D 422 36.190 35.191 100.949 1.00 57.63 O ATOM 6631 CG1 VAL D 422 38.661 36.226 102.514 1.00 58.54 C ATOM 6632 CG2 VAL D 422 39.881 37.096 102.667 1.00 60.18 C ATOM 6634 CA GLU D 423 36.646 37.343 100.455 1.00 58.12 N ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46	ATOM	6619 CA MET D 421	40.233 36.958 97.909 1.00 61.23	С
ATOM 6622 CB MET D 421 41.368 35.916 97.784 1.00 62.22 C ATOM 6623 CG MET D 421 41.916 35.960 96.369 1.00 63.61 C ATOM 6624 SD MET D 421 41.148 34.624 95.448 1.00 63.00 S ATOM 6625 CE MET D 421 42.379 33.382 95.900 1.00 65.22 C ATOM 6626 N VAL D 422 39.313 36.410 100.099 1.00 59.43 N ATOM 6627 CA VAL D 422 38.441 35.785 101.056 1.00 58.24 C ATOM 6628 C VAL D 422 36.983 36.109 100.795 1.00 57.82 C ATOM 6629 O VAL D 422 36.190 35.191 100.949 1.00 57.63 O ATOM 6630 CB VAL D 422 38.661 36.226 102.514 1.00 58.54 C ATOM 6631 CG1 VAL D 422 38.766 35.009 103.410 1.00 59.06 C ATOM 6632 CG2 VAL D 422 39.881 37.096 102.667 1.00 60.18 C ATOM 6633 N GLU D 423 36.646 37.343 100.455 1.00 58.12 N ATOM 6635 C GLU D 423 35.263 37.713 100.211 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O	ATOM	6620 C MET D 421	39.229 36.266 98.798 1.00 60.15	С
ATOM 6623 CG MET D 421 41.916 35.960 96.369 1.00 63.61 C ATOM 6624 SD MET D 421 41.148 34.624 95.448 1.00 63.00 S ATOM 6625 CE MET D 421 42.379 33.382 95.900 1.00 65.22 C ATOM 6626 N VAL D 422 39.313 36.410 100.099 1.00 59.43 N ATOM 6627 CA VAL D 422 38.441 35.785 101.056 1.00 58.24 C ATOM 6628 C VAL D 422 36.983 36.109 100.795 1.00 57.82 C ATOM 6629 O VAL D 422 36.190 35.191 100.949 1.00 57.63 O ATOM 6630 CB VAL D 422 38.661 36.226 102.514 1.00 58.54 C ATOM 6631 CG1 VAL D 422 38.766 35.009 103.410 1.00 59.06 C ATOM 6632 CG2 VAL D 422 39.881 37.096 102.667 1.00 60.18 C ATOM 6633 N GLU D 423 36.646 37.343 100.455 1.00 58.12 N ATOM 6634 CA GLU D 423 35.263 37.713 100.211 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46				
ATOM 6624 SD MET D 421 41.148 34.624 95.448 1.00 63.00 S ATOM 6625 CE MET D 421 42.379 33.382 95.900 1.00 65.22 C ATOM 6626 N VAL D 422 39.313 36.410 100.099 1.00 59.43 N ATOM 6627 CA VAL D 422 38.441 35.785 101.056 1.00 58.24 C ATOM 6628 C VAL D 422 36.983 36.109 100.795 1.00 57.82 C ATOM 6629 O VAL D 422 36.190 35.191 100.949 1.00 57.63 O ATOM 6630 CB VAL D 422 38.661 36.226 102.514 1.00 58.54 C ATOM 6631 CG1 VAL D 422 38.766 35.009 103.410 1.00 59.06 C ATOM 6632 CG2 VAL D 422 39.881 37.096 102.667 1.00 60.18 C ATOM 6633 N GLU D 423 36.646 37.343 100.455 1.00 58.12 N ATOM 6634 CA GLU D 423 35.263 37.713 100.211 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O	ATOM	6622 CB MET D 421	41.368 35.916 97.784 1.00 62.22	
ATOM 6626 N VAL D 422 39.313 36.410 100.099 1.00 59.43 N ATOM 6627 CA VAL D 422 38.441 35.785 101.056 1.00 58.24 C ATOM 6628 C VAL D 422 36.983 36.109 100.795 1.00 57.82 C ATOM 6629 O VAL D 422 36.190 35.191 100.949 1.00 57.63 O ATOM 6630 CB VAL D 422 38.661 36.226 102.514 1.00 58.54 C ATOM 6631 CG1 VAL D 422 38.766 35.009 103.410 1.00 59.06 C ATOM 6632 CG2 VAL D 422 39.881 37.096 102.667 1.00 60.18 C ATOM 6633 N GLU D 423 36.646 37.343 100.455 1.00 58.12 N ATOM 6634 CA GLU D 423 35.263 37.713 100.211 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O	ATOM	6623 CG MET D 421	41.916 35.960 96.369 1.00 63.61	С
ATOM 6626 N VAL D 422 39.313 36.410 100.099 1.00 59.43 N ATOM 6627 CA VAL D 422 38.441 35.785 101.056 1.00 58.24 C ATOM 6628 C VAL D 422 36.983 36.109 100.795 1.00 57.82 C ATOM 6629 O VAL D 422 36.190 35.191 100.949 1.00 57.63 O ATOM 6630 CB VAL D 422 38.661 36.226 102.514 1.00 58.54 C ATOM 6631 CG1 VAL D 422 38.766 35.009 103.410 1.00 59.06 C ATOM 6632 CG2 VAL D 422 39.881 37.096 102.667 1.00 60.18 C ATOM 6633 N GLU D 423 36.646 37.343 100.455 1.00 58.12 N ATOM 6634 CA GLU D 423 35.263 37.713 100.211 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O	ATOM	6624 SD MET D 421	41.148 34.624 95.448 1.00 63.00	S
ATOM 6627 CA VAL D 422 38.441 35.785 101.056 1.00 58.24 C ATOM 6628 C VAL D 422 36.983 36.109 100.795 1.00 57.82 C ATOM 6629 O VAL D 422 36.190 35.191 100.949 1.00 57.63 O ATOM 6630 CB VAL D 422 38.661 36.226 102.514 1.00 58.54 C ATOM 6631 CG1 VAL D 422 38.766 35.009 103.410 1.00 59.06 C ATOM 6632 CG2 VAL D 422 39.881 37.096 102.667 1.00 60.18 C ATOM 6633 N GLU D 423 36.646 37.343 100.455 1.00 58.12 N ATOM 6634 CA GLU D 423 35.263 37.713 100.211 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O			42.379 33.382 95.900 1.00 65.22	C
ATOM 6628 C VAL D 422 36.983 36.109 100.795 1.00 57.82 C ATOM 6629 O VAL D 422 36.190 35.191 100.949 1.00 57.63 O ATOM 6630 CB VAL D 422 38.661 36.226 102.514 1.00 58.54 C ATOM 6631 CG1 VAL D 422 38.766 35.009 103.410 1.00 59.06 C ATOM 6632 CG2 VAL D 422 39.881 37.096 102.667 1.00 60.18 C ATOM 6633 N GLU D 423 36.646 37.343 100.455 1.00 58.12 N ATOM 6634 CA GLU D 423 35.263 37.713 100.211 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O				
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ATOM 6630 CB VAL D 422 38.661 36.226 102.514 1.00 58.54 C ATOM 6631 CG1 VAL D 422 38.766 35.009 103.410 1.00 59.06 C ATOM 6632 CG2 VAL D 422 39.881 37.096 102.667 1.00 60.18 C ATOM 6633 N GLU D 423 36.646 37.343 100.455 1.00 58.12 N ATOM 6634 CA GLU D 423 35.263 37.713 100.211 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O				
ATOM 6631 CG1 VAL D 422 38.766 35.009 103.410 1.00 59.06 C ATOM 6632 CG2 VAL D 422 39.881 37.096 102.667 1.00 60.18 C ATOM 6633 N GLU D 423 36.646 37.343 100.455 1.00 58.12 N ATOM 6634 CA GLU D 423 35.263 37.713 100.211 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O				
ATOM 6632 CG2 VAL D 422 39.881 37.096 102.667 1.00 60.18 C ATOM 6633 N GLU D 423 36.646 37.343 100.455 1.00 58.12 N ATOM 6634 CA GLU D 423 35.263 37.713 100.211 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O				
ATOM 6633 N GLU D 423 36.646 37.343 100.455 1.00 58.12 N ATOM 6634 CA GLU D 423 35.263 37.713 100.211 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O		-		
ATOM 6634 CA GLU D 423 35.263 37.713 100.211 1.00 58.27 C ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O				N
ATOM 6635 C GLU D 423 34.765 36.994 98.968 1.00 55.62 C ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O				С
ATOM 6636 O GLU D 423 33.628 36.547 98.970 1.00 56.46 O				С
			33.628 36.547 98.970 1.00 56.46	
ALOM 6057 OB GEO B 125 Dick to Division Dick to	ATOM	6637 CB GLU D 423	35.048 39.198 99.981 1.00 63.42	C
ATOM 6638 CG GLU D 423 35.607 40.072 101.091 1.00 69.69 C				
ATOM 6639 CD GLU D 423 37.063 40.422 100.811 1.00 73.48 C				
ATOM 6640 OE1 GLU D 423 37.960 39.580 101.067 1.00 74.80 O	ATOM	6640 OE1 GLU D 423	37.960 39.580 101.067 1.00 74.80	U

ATOM 6642 N ILE D 424 ATOM 6643 CA ILE D 424 ATOM 6644 C ILE D 424 35.039 34.724 97.165 1.00 47.54 C 33.999 34.133 96.882 1.00 49.69 0 ATOM 6645 O ILE D 424 ATOM 6646 CB ILE D 424 36.200 36.411 95.643 1.00 46.38 ATOM 6647 CG1 ILE D 424 36.114 37.903 95.294 1.00 45.36 C C 35.964 35.578 94.409 1.00 45.99 ATOM 6648 CG2 ILE D 424 C ATOM 6649 CD1 ILE D 424 37.263 38.335 94.436 1.00 44.90 N ATOM 6650 N PHE D 425 35.937 34.114 97.908 1.00 46.05 C ATOM 6651 CA PHE D 425 35.801 32.755 98.375 1.00 46.71 C ATOM 6652 C PHE D 425 34,524 32.584 99.190 1.00 47.74 0 ATOM 6653 O PHE D 425 33.842 31.551 99.190 1.00 47.54 37.016 32.405 99.248 1.00 47.30 C ATOM 6654 CB PHE D 425 ATOM 6655 CG PHE D 425 38.166 31.801 98.512 1.00 47.90 C C 38.451 32.223 97.212 1.00 48.30 ATOM 6656 CD1 PHE D 425 ATOM 6657 CD2 PHE D 425 38,958 30.826 99.096 1.00 47.69 C C ATOM 6658 CE1 PHE D 425 39.503 31.687 96.492 1.00 47.94 C ATOM 6659 CE2 PHE D 425 40.006 30.290 98.359 1.00 49.07 C ATOM 6660 CZ PHE D 425 40.297 30.704 97.055 1.00 48.22 ATOM 6661 N ASP D 426 34.186 33.619 99.957 1.00 48.99 N 32,995 33,592 100,806 1,00 49,66 C ATOM 6662 CA ASP D 426 31.745 33.515 99.960 1.00 48.65 ATOM 6663 C ASP D 426 ATOM 6664 O ASP D 426 0 30.937 32.600 100.126 1.00 49.33 ATOM 6665 CB ASP D 426 33.068 34.750 101.780 1.00 52.02 C ATOM 6666 CG ASP D 426 33.849 34.319 103.014 1.00 54.93 C 34.046 33.091 103.166 1.00 56.47 0 ATOM 6667 OD1 ASP D 426 ATOM 6668 OD2 ASP D 426 34.255 35.179 103.836 1.00 56.41 0 31.615 34.387 98.980 1.00 46.62 N ATOM 6669 N MET D 427 30,501 34.353 98.054 1.00 45.37 C ATOM 6670 CA MET D 427 C ATOM 6671 C MET D 427 30.453 33.005 97.344 1.00 44.51 0 29.396 32.363 97.184 1.00 44.03 ATOM 6672 O MET D 427 ATOM 6673 CB MET D 427 30,694 35.519 97.101 1.00 45.87 C 30.450 36.824 97.861 1.00 47.01 C ATOM 6674 CG MET D 427 30.460 38.224 96.731 1.00 49.65 S ATOM 6675 SD MET D 427 C 32.203 38.257 96.268 1.00 49.56 ATOM 6676 CE MET D 427 N ATOM 6677 N LEU D 428 31.633 32.531 96.925 1.00 42.70 ATOM 6678 CA LEU D 428 31.688 31.231 96.268 1.00 41.62 C 31.151 30.140 97.192 1.00 41.91 С ATOM 6679 C LEU D 428 ATOM 6680 O LEUD 428 30.313 29.314 96.779 1.00 42.48 0 C ATOM 6681 CB LEUD 428 33.070 30.931 95.734 1.00 39.31 33.510 31.798 94.557 1.00 38.32 C ATOM 6682 CG LEU D 428 35.002 31.635 94.331 1.00 38.19 C ATOM 6683 CD1 LEU D 428 C 32.761 31.369 93.301 1.00 39.42 ATOM 6684 CD2 LEU D 428

31.572 30.144 98.456 1.00 41.27

N

ATOM 6685 N LEU D 429

wo	98/56812	258/371	PCT/GB98/01708
ATOM	6686 CA 1 FUD 429	31.106 29.081 99.350 1.00 40.57	C
		29.624 29.149 99.574 1.00 40.99	
ATOM	6688 O LEUD 429	28.927 28.132 99.528 1.00 42.18	0
ATOM	6689 CB LEU D 429	31.940 29.105 100.603 1.00 40.44	С
ATOM	6690 CG LEUD 429	33.393 28.673 100.380 1.00 39.94	С
ATOM	6691 CD1 LEU D 429	34.220 29.148 101.544 1.00 41.13	C
ATOM	6692 CD2 LEU D 429	33.455 27.174 100.190 1.00 39.25	С
		29.084 30.334 99.778 1.00 40.85	
ATOM	6694 CA ALAD 430	27.658 30.515 99.970 1.00 40.65	
ATOM	6693 C ALAD 430	26.865 30.012 98.778 1.00 42.44 25.754 29.491 98.938 1.00 45.02	C O
		27.394 32.002 100.090 1.00 40.90	
ATOM	6698 N THR D 431	27 339 30 174 97 548 1 00 41 99	N
ATOM	6699 CA THR D 431	27.339 30.174 97.548 1.00 41.99 26.562 29.674 96.429 1.00 41.67	C
ATOM	6700 C THR D 431	26.632 28.170 96.457 1.00 42.17	C
		25.698 27.427 96.233 1.00 42.18	
ATOM	6702 CB THR D 431	27.210 30.134 95.114 1.00 42.80	С
ATOM	6703 OG1 THR D 431	27.425 31.538 95.287 1.00 43.83 26.328 29.798 93.924 1.00 42.25	0
ATOM	6704 CG2 THR D 431	26.328 29.798 93.924 1.00 42.25	С
		27.845 27.694 96.722 1.00 43.94	
ATOM	6706 CA SER D 432	28.113 26.258 96.733 1.00 45.18	C
ATOM	6707 C SER D 432	27.161 25.571 97.694 1.00 45.21 26.566 24.533 97.490 1.00 44.06	C
ATOM	6700 CR SER D 432	29.597 26.004 97.039 1.00 44.71	0
		29.733 24.588 96.992 1.00 46.22	
		27.009 26.186 98.839 1.00 46.87	
ATOM	6712 CA SER D 433	26.148 25.773 99.910 1.00 49.54	C
		24.695 25.808 99.488 1.00 50.44	
ATOM	6714 O SER D 433	23.986 24.827 99.672 1.00 51.36	0
ATOM	6715 CB SER D 433	26.388 26.859 100.967 1.00 51.99 25.889 26.318 102.168 1.00 56.70	С
	6717 N ARG D 434	24.230 26.902 98.878 1.00 50.98	N
	6718 CA ARG D 434		С
	6719 C ARG D 434	22.667 25.859 97.401 1.00 51.71	С
	6720 O ARG D 434 6721 CB ARG D 434	21.629 25.218 97.447 1.00 51.99 22.500 28.356 97.835 1.00 52.96	O C
	6722 CG ARG D 434	21.112 28.377 97.229 1.00 55.73	C
	6723 CD ARG D 434		č
	6724 NE ARG D 434	18.818 29.386 97.162 1.00 61.34	N
	6725 CZ ARG D 434	18.049 28.559 97.888 1.00 62.31	C
ATOM	6726 NH1 ARG D 434	18.586 27.916 98.937 1.00 63.44	N
	6727 NH2 ARG D 434	16.779 28.329 97.626 1.00 62.37	N
	6728 N PHE D 435	23.601 25.561 96.505 1.00 53.07	N
•	6729 CA PHE D 435	23.390 24.473 95.565 1.00 55.49	C
ATOM	6730 C PHE D 435	23.233 23.160 96.327 1.00 56.68	С

WO 98/56812

wo	98/56812	260/371	PCT/GB98/01708
4 TO 1 4	6776 C LEU D 440	21.482 19.488 91.649 1.00 59.80	С
		22.502 18.898 91.974 1.00 59.93	Ö
ATOM	6778 CR 1 FILD 440	21.877 21.934 92.171 1.00 57.04	C
ATOM	6779 CG LEUD 440	22.209 22.280 90.727 1.00 55.79	Č
ATOM	6780 CD1 I FU D 440	20.992 22.898 90.077 1.00 55.60	C
ATOM	6781 CD2 I FII D 440	23.398 23.211 90.649 1.00 56.07	Č
		20.729 19.111 90.627 1.00 60.60	N
ATOM	6783 CA GIND 441	21.067 17.981 89.792 1.00 61.02	
ATOM	6784 C GIND 441	22.036 18.348 88.699 1.00 59.67	C
ATOM	6785 O GIND 441	22.047 19.490 88.298 1.00 60.79	Ö
ATOM	6786 CP GIND 441	19.784 17.547 89.071 1.00 63.67	
ATOM	6787 CG GIND 441	18 746 16 948 89 995 1 00 67 17	
ATOM	6788 CD GIND 441	18.746 16.948 89.995 1.00 67.17 19.375 16.015 91.025 1.00 69.21	Ċ
ATOM	6780 OFI GIND 441	19.706 14.899 90.611 1.00 70.52	Ō
ATOM	6790 NE2 GLN D 441	19.536 16.461 92.274 1.00 69.73	N
ATOM	6791 N GLYD 442	22.784 17.416 88.158 1.00 59.13	N
		23.713 17.697 87.078 1.00 56.87	C
		22.979 18.101 85.824 1.00 56.45	C
		23.546 18.922 85.108 1.00 56.38	
ATOM	6795 N GLUD 443	21.780 17.593 85.534 1.00 56.59	
ATOM	6796 CA GLUD 443	21.083 18.001 84.315 1.00 57.10	С
ATOM	6797 C GLUD 443	20.719 19.479 84.468 1.00 54.01	С
ATOM	6798 O GLUD 443	20.759 20.200 83.499 1.00 53.31	0
ATOM	6799 CB GLU D 443	19.818 17.241 83.962 1.00 61.47	С
ATOM	6800 CG GLU D 443	19.787 15.730 83.877 1.00 64.56	С
ATOM	6801 CD GLU D 443	20.350 15.084 85.131 1.00 66.39	C
ATOM	6802 OE1 GLU D 443	20.020 15.514 86.252 1.00 67.30	0
ATOM	6803 OE2 GLU D 443	21.152 14.148 84.960 1.00 67.90	0
ATOM	6804 N GLUD 444	20.362 19.872 85.680 1.00 51.49	N
		20.031 21.253 85.994 1.00 48.76	С
	6806 C GLU D 444		С
<b>ATOM</b>	6807 O GLU D 444	21.284 23.084 85.088 1.00 48.04	0
		19.563 21.350 87.437 1.00 48.48	С
<b>ATOM</b>	6809 CG GLU D 444	18.148 20.791 87.568 1.00 48.45	С
		17.672 20.825 89.007 1.00 48.07	С
<b>ATOM</b>	6811 OEI GLU D 444	18.484 20.503 89.894 1.00 46.60	0
ATOM	6812 OE2 GLU D 444	16.487 21.181 89.132 1.00 48.63	Ο
	6813 N PHE D 445	22.367 21.654 86.413 1.00 45.51	N
	6814 CA PHE D 445	23.650 22.321 86.311 1.00 44.62	С
	6815 C PHE D 445	23.980 22.706 84.875 1.00 44.77	C
	6816 O PHE D 445	24.234 23.841 84.512 1.00 45.62	0
		24.794 21.461 86.864 1.00 43.02	C
	6818 CG PHE D 445	26.158 21.994 86.559 1.00 41.95	C
		26.552 23.244 86.990 1.00 42.64	C
ATOM	6820 CD2 PHE D 445	27.057 21.271 85.831 1.00 41.88	С

	98/568		261/371	PCT/GB98/01708
ATOM	6921	CEI DHE D 445	27.795 23.757 86.729 1.00 42.63 28.325 21.740 85.532 1.00 41.96 28.683 22.990 85.987 1.00 43.00	С
ATOM	6822	CE2 PHF D 445	28 325 21 740 85 532 1 00 41.96	Č
ATOM	6823	CZ PHE D 445	28.683 22.990 85.987 1.00 43.00	C
ATOM	6824	N VAL D 446	24.011 21.738 84.006 1.00 44.75	N
ATOM	6825	CA VAL D 446	24.323 21.845 82.595 1.00 44.55	С
ATOM	6826	C VAL D 446	24.323 21.845 82.595 1.00 44.55 23.423 22.850 81.915 1.00 45.82	С
ATOM	6827	O VAL D 446	23.856 23.614 81.021 1.00 46.31	O
ATOM	6828	CB VAL D 446	24.348 20.374 82.130 1.00 43.66	С
<b>ATOM</b>	6829	CG1 VAL D 446	23.502 20.001 80.941 1.00 43.51 25.797 20.021 81.897 1.00 43.07	С
<b>ATOM</b>	6830	CG2 VAL D 446	25.797 20.021 81.897 1.00 43.07	С
ATOM	6831	N CYS D 447	22.153 22.923 82.294 1.00 46.23	N
<b>ATOM</b>	6832	CA CYS D 447	21.235 23.886 81.701 1.00 47.72	С
<b>ATOM</b>	6833	C CYS D 447	21.530 25.334 82.093 1.00 47.52 21.531 26.206 81.246 1.00 46.80 19.827 23.550 82.214 1.00 48.91	С
ATOM	6834	O CYS D 447	21.531 26.206 81.246 1.00 46.80	0
ATOM	6835	CB CYS D 447	19.827 23.550 82.214 1.00 48.91	C
ATOM	6836	SG CYS D 447	18.991 22.336 81.203 1.00 50.22	S
ATOM	6837	N LEU D 448	21.738 25.570 83.391 1.00 46.99 22.070 26.868 83.934 1.00 45.68	N
ATOM	6838	CA LEU D 448	22.070 26.868 83.934 1.00 45.68	C
ATOM	6839	C LEU D 448	23.332 27.419 83.290 1.00 44.95	C
			23.429 28.572 82.884 1.00 45.79	
ATOM	6841	CB LEU D 448	22.314 26.760 85.434 1.00 45.92	C
ATOM	6842	CG LEU D 448	21.093 26.655 86.347 1.00 45.80 21.617 26.450 87.757 1.00 46.68 20.193 27.878 86.304 1.00 44.62	C
ATOM	6843	CD1 LEU D 448	21.017 20.430 87.737 1.00 40.00	C
ATOM	6015	N I VC D 440	24.331 26.561 83.154 1.00 44.17	N
ATOM	6945	CA IVED 449	25.599 26.948 82.536 1.00 43.37	C
ATOM	6947	C 1 V 5 D 440	25.338 27.458 81.139 1.00 42.62	c
ATOM	6848	O IVSD 449	25.877 28.518 80.806 1.00 43.03	Ö
ATOM	6849	CR LYS D 449	26.554 25.791 82.659 1.00 43.95	C
ATOM	6850	CG LYS D 449	28.009 26.153 82.807 1.00 44.50	С
ATOM	6851	CD LYS D 449	28.009 26.153 82.807 1.00 44.50 28.769 25.193 81.908 1.00 45.79	C
ATOM	6852	CE LYS D 449	29,224 23.981 82.706 1.00 46.49	С
		NZ LYS D 449	30.163 23.282 81.735 1.00 49.77	N
<b>ATOM</b>	6854	N SER D 450	24.512 26.815 80.322 1.00 42.15	N
<b>ATOM</b>	6855	CA SER D 450	24.238 27.374 78.992 1.00 41.89	C
<b>ATOM</b>	6856	C SER D 450	23.410 28.642 79.057 1.00 40.65	С
<b>ATOM</b>	6857	O SER D 450	23.605 29.481 78.202 1.00 41.51	0
		CB SER D 450	23.432 26.431 78.101 1.00 42.84	<b>C</b>
		OG SER D 450	24.173 25.209 78.223 1.00 46.38	0
		N ILE D 451	22.513 28.790 80.017 1.00 39.36	N
		CA ILED 451	21.698 29.976 80.148 1.00 37.93	C
		C ILED 451	22.686 31.110 80.369 1.00 37.94	С
		O ILE D 451	22.518 32.116 79.704 1.00 37.47	0
			20.725 29.872 81.329 1.00 38.37	C C
ATOM	6865	CG1 ILE D 451	19.741 28.776 80.952 1.00 38.67	C

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АТОМ	6866 CG2 ILE D 451	20.093 31.213 81.662 1.00 37.38	C
ATOM	6867 CD1 ILE D 451	18.514 28.737 81.822 1.00 41.51	Ċ
ATOM	6868 N ILE D 452	23.676 30.877 81.240 1.00 37.60	N
<b>ATOM</b>	6869 CA ILE D 452	24.691 31.886 81.525 1.00 36.56	С
ATOM	6870 C ILE D 452	25.436 32.257 80.256 1.00 36.13	C
ATOM	6871 O ILE D 452	25.610 33.434 80.030 1.00 36.37 25.730 31.436 82.579 1.00 35.77	0
ATOM	6872 CB ILE D 452	25.730 31.436 82.579 1.00 35.77	C C
		25.014 31.155 83.900 1.00 34.24 26.844 32.461 82.723 1.00 34.78	
ATOM	6875 CD1 ILE D 452	25 892 30 989 85 099 1 00 33 24	C
ATOM	6876 N LEU D 453	25.892 30.989 85.099 1.00 33.24 25.838 31.286 79.452 1.00 36.42	N
ATOM	6877 CA LEUD 453	26.549 31.553 78.228 1.00 36.94	С
ATOM	6878 C LEU D 453	25.696 32.400 77.310 1.00 38.42	С
ATOM	6879 O LEU D 453	26.173 33.323 76.682 1.00 39.35 26.968 30.277 77.478 1.00 35.54	Ο
ATOM	6880 CB LEU D 453	26.968 30.277 77.478 1.00 35.54	C
		27.531 30.530 76.067 1.00 35.05	
		28.844 31.294 76.058 1.00 33.75	
	6884 N LEU D 454	27.718 29.250 75.299 1.00 34.02 24.431 32.083 77.160 1.00 41.14	N
		23.570 32.821 76.262 1.00 43.55	
		22.976 34.121 76.765 1.00 44.50	
ATOM	6887 O LEUD 454	22.805 35.002 75.913 1.00 46.40	0
ATOM	6888 CB LEU D 454	22.380 31.917 75.839 1.00 43.39	С
ATOM	6889 CG LEU D 454	22.823 30.835 74.849 1.00 43.72	С
		21.789 29.750 74.787 1.00 44.06	
		23.000 31.428 73.468 1.00 44.69	
	6892 N ASN D 455		N
		21.990 35.492 78.456 1.00 45.22 22.911 36.573 78.923 1.00 48.85	
		22.447 37.720 78.958 1.00 51.01	
		21.026 35.166 79.579 1.00 44.21	C
	6897 CG ASN D 455	20.481 36.271 80.419 1.00 43.95	С
	6898 OD1 ASN D 455	20.909 36.409 81.568 1.00 44.44	O
	6899 ND2 ASN D 455	19.557 37.057 79.888 1.00 43.94	N
	6900 N SER D 456	24.141 36.290 79.297 1.00 52.15	N
	6901 CA SER D 456	24.949 37.375 79.841 1.00 55.13	C
	6902 C SER D 456	25.284 38.474 78.866 1.00 57.33 25.192 39.676 79.158 1.00 58.90	C O
	6903 O SER D 456 6904 CB SER D 456	26.177 36.767 80.523 1.00 55.03	C
	6905 OG SER D 456	25.851 36.397 81.835 1.00 53.67	Ö
	6906 N GLY D 457	25.695 38.152 77.664 1.00 59.87	N
	6907 CA GLY D 457	26.071 39.211 76.728 1.00 63.73	C
ATOM	6908 C GLY D 457	24.984 39.616 75.764 1.00 65.27	С
	6909 O GLY D 457	25,290 40,349 74,835 1.00.64.43	0
ATOM	6910 N VAL D 458	23.767 39.137 75.986 1.00 68.09	N

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		22.681 39.469 75.080 1.00 71.03	С
	6912 C VAL D 458		C
	6913 O VAL D 458		0
		21.475 38.547 75.320 1.00 69.39	С
ATOM	6915 CG1 VAL D 458	20.688 38.875 76.549 1.00 68.27	С
ATOM	6916 CG2 VAL D 458	20.585 38.594 74.081 1.00 69.67	С
ATOM	6917 N TYR D 459	22.356 41.782 75.995 1.00 78.79	N
ATOM	6918 CA TYR D 459	22.008 43.181 75.933 1.00 83.41	С
ATOM	6919 C TYR D 459	23.164 44.036 75.477 1.00 85.77	С
ATOM	6920 O TYR D 459	23.175 45.241 75.717 1.00 87.22	0
ATOM	6921 CB TYR D 459	21.561 43.737 77.319 1.00 85.69	С
ATOM		20.493 42.800 77.854 1.00 87.98	С
ATOM	6923 CD1 TYR D 459	20.862 41.683 78.595 1.00 88.70	С
ATOM	6924 CD2 TYR D 459	19.147 43.003 77.594 1.00 88.99	С
		19.896 40.820 79.060 1.00 90.23	С
		18.177 42.130 78.049 1.00 90.00	С
		18.552 41.030 78.792 1.00 90.79	С
<b>ATOM</b>		17.609 40.133 79.271 1.00 91.09	Ο
<b>ATOM</b>			N
<b>ATOM</b>	6930 CA THR D 460	25.327 44.222 74.394 1.00 90.99	С
<b>ATOM</b>			C
<b>ATOM</b>	6932 O THR D 460	27.027 43.515 72.869 1.00 93.66	0
ATOM	6933 CB THR D 460		C
ATOM			0
<b>ATOM</b>	6935 CG2 THR D 460		С
ATOM			N
ATOM	6937 CA PHE D 461	25.314 42.844 70.878 1.00 94.98	С
<b>ATOM</b>			C
<b>ATOM</b>			0
		24.119 42.166 70.170 1.00 94.65	C
		24.263 40.679 70.430 1.00 93.76	· C
ATOM		25.524 40.137-70.616 1.00 93.43	·C
ATOM	6943 CD2 PHE D 461	23.176 39.849 70.503 1.00 93.49	C
	6944 CE1 PHE D 461	25.726 38.809 70.870 1.00 93.10	C
	6945 CE2 PHE D 461	23.368 38.511 70.750 1.00 93.62	C
	6946 CZ PHE D 461	24.631 37.983 70.932 1.00 93.40	С
	6947 N THR D 465	22.624 45.967 63.550 1.00127.65	N
	6948 CA THR D 465	21.376 46.227 64.267 1.00127.69	C
ATOM		20.289 45.238 63.883 1.00126.64	C
ATOM		19,950 44.353 64.675 1.00127.34	.0
ATOM		20.851 47.661 64.084 1.00128.43	C
	6952 OG1 THR D 465	19,424 47.705 64.272 1.00128.82	0
	6953 CG2 THR D 465	21.170 48.197 62.693 1.00128.79	C
ATOM	6954 N LEUD 466	19.741 45.302 62.672 1.00124.51	N
ATOM	6955 CA LEU D 466	18.705 44.356 62.251 1.00122.04	С

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<b>ATOM</b>	6956 C LEU D 466	19.174 42.908 62.392 1.00119.80	С
		18.380 42.001 62.689 1.00119.83	
<b>ATOM</b>	6958 CB LEUD 466	18.239 44.686 60.837 1.00122.41	C
<b>ATOM</b>	6962 N LYS D 467	20.472 42.656 62.200 1.00116.36	N
<b>ATOM</b>	6963 CA LYS D 467	21.041 41.328 62.370 1.00112.85	С
<b>ATOM</b>	6964 C LYS D 467	21.062 41.103 63.887 1.00108.83	С
<b>ATOM</b>	6965 O LYS D 467	20.845 39.985 64.333 1.00108.82	0
<b>ATOM</b>	6966 CB LYS D 467	22.439 41.155 61.790 1.00114.37	C
ATOM	6967 CG LYS D 467	22.851 39.725 61.452 1.00115.62	С
ATOM	6968 CD LYS D 467	24.347 39.658 61.199 1.00117.19	С
<b>ATOM</b>	6969 CE LYS D 467	24.756 39.606 59.729 1.00117.88	С
		26.238 39.769 59.560 1.00117.63	
	6971 N SER D 468	21.292 42.150 64.670 1.00103.70	
		21.303 42.054 66.114 1.00 99.58	
		19.922 41.722 66.669 1.00 96.01	
		19.782 40.953 67.608 1.00 95.40	
ATOM	6975 CB SER D 468	21.709 43.362 66.797 1.00100.34	С
ATOM	6976 OG SER D 468	23.064 43.653 66.528 1.00101.77	0
		18.903 42.320 66.067 1.00 92.13	N
		17.527 42.083 66.486 1.00 88.58	
		17.207 40.624 66.216 1.00 86.29	
		16.507 39.969 66.976 1.00 85.00	0
		16.606 43.082 65.801 1.00 89.09	
		17.735 40.088 65.119 1.00 84.72	
ATOM	6986 CA GLUD 470	17.526 38.684 64.759 1.00 83.02	C
		18.373 37.818 65.673 1.00 78.98	
		17.939 36.776 66.149 1.00 77.81	
ATOM	6989 CB GLUD 470	17.772 38.529 63.280 1.00 87.02	C C
ATOM	6990 CG GLUD 470	18.612 37.362 62.816 1.00 92.72 19.073 37.527 61.375 1.00 96.70	C
ATOM	6992 OE1 GLU D 470	18.960 38.661 60.822 1.00 98.66	0
	6993 OE2 GLU D 470	19.551 36.519 60.786 1.00 98.72	O
	6994 N GLUD 471	19.596 38.228 65.989 1.00 75.15	N
	6995 CA GLUD 471	20.506 37.543 66.889 1.00 70.77	Ċ
	6996 C GLU D 471	19.871 37.513 68.283 1.00 69.37	c
	6997 O GLUD 471	19.873 36.498 68.972 1.00 68.92	Ö
	6998 CB GLU D 471	21.863 38.216 66.977 1.00 69.02	C
	6999 CG GLU D 471	22.727 38.202 65.767 1.00 67.63	Ċ
	7000 CD GLUD 471	23.780 37.140 65.725 1.00 68.27	Č
	7001 OE1 GLU D 471	24.767 37.192 66.463 1.00 67.40	O
	7002 OE2 GLU D 471	23.681 36.173 64.932 1.00 69.91	0
	7003 N LYS D 472	19.311 38.636 68.724 1.00 68.00	N
	7004 CA LYS D 472	18.643 38.704 70.011 1.00 66.62	С
ATOM	7005 C LYS D 472	17.455 37.755 70.031 1.00 64.90	С
ATOM	7006 O LYS D 472	17.316 37.050 71.014 1.00 65.02	O

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<b>ATOM</b>	7007 CB LYS D 472	18 168 40.104 70.395 1.00 67.81	C
ATOM	7008 CG LYS D 472	19.292 41.038 70.752 1.00 70.56	C
ATOM	7009 CD LYS D 472	18.827 42.323 71.380 1.00 73.00	C
ATOM	7010 CE LYS D 472	19.691 43.522 71.019 1.00 75.44	С
ATOM	7011 NZ LYS D 472	20.894 43.754 71.896 1.00 77.11	N
		16.602 37.676 69.030 1.00 64.19	
ATOM	7013 CA ASP D 473	15.466 36.783 69.058 1.00 64.15	C
ATOM	7014 C ASP D 473	15.899 35.335 69.128 1.00 61.42	C
ATOM	7015 O ASP D 473	15.385 34.559 69.902 1.00 62.62	0
ATOM	7016 CB ASP D 473	14.611 36.829 67.796 1.00 68.83 13.999 38.198 67.618 1.00 73.25	C
ATOM	7017 CG ASP D 473	13.999 38.198 67.618 1.00 73.25	С
ATOM	7018 OD1 ASP D 473	14.079 39.069 68.518 1.00 75.35	
ATOM	7019 OD2 ASP D 473	13.409 38.384 66.527 1.00 76.20	.0
		16.838 34.967 68.286 1.00 57.77	N
ATOM	7021 CA HIS D 474	17.345 33.610 68.285 1.00 54.52	С
ATOM	7022 C HIS D 474	17.726 33.238 69.714 1.00 53.80	C
ATOM	7023 O HIS D 474	17.292 32.240 70.293 1.00 52.80	0
ATOM	7024 CB HIS D 474	18.570 33.612 67.358 1.00 53.69	C
ATOM	7025 CG HIS D 474	19.062 32.195 67.328 1.00 53.28	C
ATOM	7026 ND1 HIS D 474	18.207 31.170 66.988 1.00 52.17	N
ATOM	7027 CD2 HIS D 474	20.267 31.676 67.651 1.00 53.88	C
ATOM	7028 CE1 HIS D 474	18.892 30.051 67.065 1.00 53.66	C
ATOM	7029 NE2 HIS D 474	20.131 30.321 67.468 1.00 54.49	N
ATOM	7030 N ILE D 475	18.586 34.047 70.342 1.00 53.00	N
ATOM	7031 CA ILE D 475	19.002 33.822 71.705 1.00 52.51	С
ATOM	7032 C ILED 475	17.794 33.715 72.609 1.00 52.34	C
ATOM	7033 O ILED 475	17.680 32.717 73.325 1.00 51.65	0
ATOM	7034 CB ILE D 475	19.957, 34.910, 72.201, 1.00, 53.42	C C
ATOM	7035 CGI ILE D 475	21.273 34.733 71.434 1.00 53.48	C
ATOM	7036 CG2 ILE D 475	20.174 34.816 73.709 1.00 53.71 22.329 35.716 71.891 1.00 53.61	C
ATOM	7037 CDI ILE D 475	16 995 24 674 72 601 1 00 53 92	. N
		16.885 34.674 72.601 1.00 53.82 15.700 34.570 73.454 1.00 56.40	C
ATOM	7039 CA HIS D 476	14.964 33.260 73.213 1.00 57.06	c
	7040 C HIS D 476 7041 O HIS D 476	14.536 32.605 74.163 1.00 57.87	0
	7042 CB HIS D 476	14.776 35.765 73.299 1.00 58.36	C
	7043 CG HIS D 476	15.381 36.987 73.932 1.00 59.96	C
	7044 ND1 HIS D 476	15.964 36.937 75.168 1.00 60.20	N .
	7045 CD2 HIS D 476	15,490 38.263 73.490 1.00 60.94	C
	7046 CE1 HIS D 476	16.414 38.150 75.448 1.00 61.50	č
		16.146 38.983 74.461 1.00 60.99	N
	7047 NE2 HIS D 476 7048 N ARG D 477	14.814 32.815 71.987 1.00 50.39	N
	7049 CA ARG D 477	14.197 31.586 71.587 1.00 57.91	C
	7050 C ARG D 477	14.841 30.342 72.177 1.00 56.02	c
		14.134 29.464 72.665 1.00 56.11	0
ATOM	7051 O ARG D 477	14.134 29.404 72.003 1.00 30.11	J

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ATOM	7052 CB ARG D 477	14.316 31.406 70.069 1.00 62.44	C
ATOM	7053 CG ARG D 477	13.037 30.852 69.468 1.00 67.89	C
ATOM	7054 CD ARG D 477	12.106 32.067 69.294 1.00 73.64	C
ATOM	7055 NE ARG D 477	12.755 32.943 68.307 1.00 79.62	N
		12.723 32.654 66.993 1.00 82.77	
ATOM	7057 NH1 ARG D 477	12.074 31.552 66.581 1.00 84.58	
		13.327 33.463 66.125 1.00 83.31	N
ATOM	7059 N VAL D 478	16.164 30.245 72.108 1.00 53.51	N
ATOM	7060 CA VAL D 478	16.899 29.103 72.662 1.00 50.86	C
ATOM	7061 C VAL D 478	16.752 29.150 74.171 1.00 49.96	C
	7062 O VAL D 478	16.558 28.175 74.891 1.00 50.09	0
ATOM		18.382 29.178 72.250 1.00 50.20	C
ATOM	7064 CG1 VAL D 478	19.216 28.029 72.758 1.00 48.27	C
		18.446 29.262 70.725 1.00 50.29	C
		16.795 30.363 74.733 1.00 48.62	N
		16.616 30.525 76.169 1.00 47.30	С
ATOM	7068 C LEU D 479	15.276 29.961 76.605 1.00 48.58	C
ATOM	7069 O LEU D 479	15.220 29.398 77.701 1.00 49.89	0
ATOM	7070 CB LEU D 479	16.775 31.980 76.570 1.00 44.30 18.221 32.407 76.806 1.00 41.99	C
ATOM	7071 CG LEUD 479	18.221 32.407 76.806 1.00 41.99	C C
		18.316 33.919 76.921 1.00 41.99	C
		18.795 31.728 78.021 1.00 40.35	N
		14.210 30.084 75.818 1.00 49.32	C
		12.914 29.543 76.184 1.00 48.95	c
		12.997 28.035 76.109 1.00 49.02 12.503 27.345 76.972 1.00 48.57	Ö
ATOM	7079 CD ACD D 480	11.818 30.030 75.284 1.00 50.60	C
ATOM	7070 CG ASP D 480	11.434 31.479 75.430 1.00 52.07	
ATOM	7090 OD1 ASP D 480	11.626 32.083 76.497 1.00 52.84	O
ATOM	7081 OD2 ASP D 480	10.914 32.052 74.437 1.00 53.13	Ö
		13.653 27.514 75.096 1.00 51.64	N
	7083 CA LYS D 481		С
	7084 C LYS D 481		С
	7085 O LYS D 481		0
	7086 CB LYS D 481	14.582 25.684 73.664 1.00 56.66	С
	7087 CG LYS D 481		С
	7088 CD LYS D 481	13.285 23.957 72.380 1.00 65.28	С
	7089 CE LYS D 481	12.750 22.535 72.454 1.00 67.98	С
		12.998 21.867 73.776 1.00 70.18	N
	7091 N ILE D 482	15.627 26.170 76.564 1.00 50.96	N
	7092 CA ILE D 482	16.337 25.699 77.749 1.00 49.43	С
	7093 C ILE D 482	15.423 25.802 78.951 1.00 48.89	С
<b>ATOM</b>	7094 O ILE D 482	15.434 24.924 79.824 1.00 49.34	О
		17.681 26.367 77.979 1.00 49.26	С
ATOM	7096 CG1 ILE D 482	18.611 26.001 76.815 1.00 49.57	С

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ATOM	7097	CG2 ILE D 482	18.331 25.915 79.270 1.00 48.99	С
ATOM	7098	CD1 ILE D 482	19.441 27.195 76.405 1.00 49.58	
ATOM			14.572 26.816 79.034 1.00 48.55	N
ATOM			13.648 26.883 80.168 1.00 48.75	С
ATOM	7101	C THR D 483	12.727 25.666 80.165 1.00 49.97	С
ATOM	7102	O THR D 483	12.480 25.027 81.188 1.00 50.53	O
ATOM	7103	CB THR D 483	12.796 28.149 80.107 1.00 47.82	С
			13.740 29.204 80.281 1.00 48.13	Ο
ATOM	7105	CG2 THR D 483	11.734 28.119 81.182 1.00 47.64	С
<b>ATOM</b>	7106	N ASP D 484	12.221 25.336 78.964 1.00 49.96	N
<b>ATOM</b>	7107	CA ASP D 484	11.329 24.201 78.824 1.00 48.69	С
<b>ATOM</b>			12.055 22.962 79.277 1.00 48.48	C
ATOM	7109	O ASP D 484	11.484 22.156 80.010 1.00 50.20	0
ATOM	7110	CB ASP D 484	10.818 24.054 77.419 1.00 49.22	C
ATOM	7111	CG ASP D 484	9.855 25.145 77.025 1.00 50.77	C
ATOM	7112	OD1 ASP D 484	9.301 25.870 77.886 1.00 50.61 9.653 25.271 75.789 1.00 52.45	0
ATOM	7113	OD2 ASP D 484	9,653 25,271 75,789 1.00 52,45	O N
ATOM	7114	N THR D 485	13.310 22.799 78.886 1.00 47.73	
ATOM	7115	CA THR D 485	14.055 21.610 79.302 1.00 47.22	C
ATOM	/116	C THR D 485	14.152 21.504 80.810 1.00 48.41 14.057 20.420 81.374 1.00 48.46	0
ATOM	7110	CD TIM D 485	15.460 21.727 78.713 1.00 45.73	C
ATOM	7110	OCI TUD D 485	15.224 21.938 77.324 1.00 45.98	o
ATOM	7120	CG2 THP D 485	16.242 20.496 79.033 1.00 45.10	Č
ATOM	7120	N I FII D 486	14.336 22.652 81.464 1.00 48.84	N
ATOM	7121	CA I FII D 486	14.445 22.680 82.908 1.00 49.26	C
ATOM	7122	C LELID 486	13.173 22.222 83.594 1.00 50.81	
ATOM	7124	O LEUD 486	13.225 21.422 84.521 1.00 50.74	0
ATOM	7125	CB LEU D 486	14.766 24.095 83.387 1.00 47.63	С
ATOM	7126	CG LEU D 486	16.242 24.335 83.695 1.00 46.21	С
ATOM	7127	CD1 LEU D 486	16.377 25.792 84.101 1.00 46.08	С
ATOM	7128	CD2 LEU D 486	16.818 23.376 84.714 1.00 43.41	<b>C</b> .
		N ILE D 487	12.031 22.742 83.137 1.00 52.73	N
		CA ILE D 487	10.736 22.360 83.707 1.00 53.30	C
		C ILE D 487	10.511 20.882 83.456 1.00 54.63	C
		O ILE D 487	10.065 20.157 84.323 1.00 54.41	0
		CB ILE D 487	9.598 23.141 83.053 1.00 52.55	C
		CG1 ILE D 487	9.676 24.593 83.491 1.00 53.86	C
		CG2 ILE D 487	8.283 22.509 83.415 1.00 53.12	C C
		CD1 ILE D 487	9.134 24.958 84.855 1.00 52.98	N
		N HIS D 488	10.857 20.468 82.238 1.00 57.04	C
		CA HIS D 488	10.720 19.085 81.829 1.00 59.25 11.406 18.179 82.838 1.00 58.05	c
		C HIS D 488 O HIS D 488	10.892 17.222 83.368 1.00 57.71	o
		CB HIS D 488	11.346 18.872 80.448 1.00 62.29	C
ATOM	/ 141	CD FILS D 400	11.540 10.072 00.440 1.00 02.25	_

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ATOM	7142 CG HIS D 488	11.405 17.399 80.140 1.00 65.17	С
ATOM	7143 ND1 HIS D 488	10.283 16.647 79.880 1.00 66.20	N
ATOM	7144 CD2 HIS D 488	12.478 16.572 80.079 1.00 66.45	С
ATOM	7145 CE1 HIS D 488	10 692 15 405 79 660 1.00 67.99	С
ATOM	7146 NE2 HIS D 488	12.020 15.318 79.775 1.00 67.51	N
ATOM	7147 N LEUD 489	12.657 18.487 83.108 1.00 57.87	N
ATOM	7148 CA LEUD 489	13.449 17.742 84.055 1.00 57.53	С
ATOM	7149 C LEUD 489	12.778 17.642 85.404 1.00 58.23	С
ATOM	7150 O LEUD 489	12.730 16.581 85.998 1.00 59.34	0
ATOM	7151 CB LEU D 489	14.777 18.483 84.230 1.00 57.04	С
ATOM	7152 CG LEU D 489	15.786 18.189 83.137 1.00 57.56	С
ATOM	7153 CD1 LEU D 489	16.973 19.125 83.290 1.00 58.88	C
ATOM	7154 CD2 LEU D 489	16.267 16.752 83.176 1.00 57.38	C
ATOM	7155 N MET D 490	12.284 18.722 85.953 1.00 59.22	N
ATOM	7156 CA MET D 490	11.641 18.827 87.233 1.00 59.67	· C
<b>ATOM</b>	7157 C MET D 490	10.329 18.068 87.318 1.00 60.84	С
<b>ATOM</b>	7158 O MET D 490	10.051 17.498 88.371 1.00 61.71	0
ATOM	7159 CB MET D 490	11.319 20.304 87.492 1.00 59.79	С
<b>ATOM</b>	7160 CG MET D 490	12.404 21.038 88.234 1.00 59.24 12.190 22.803 88.134 1.00 57.81	С
<b>ATOM</b>	7161 SD MET D 490	12.190 22.803 88.134 1.00 57.81	S
ATOM	7162 CE MET D 490	13.863 23.335 87.948 1.00 59.41	С
<b>ATOM</b>	7163 N ALA D 491	9,549 18.101 86.237 1.00 61.24	N
ATOM	7164 CA ALA D 491	8.278 17.372 86.247 1.00 61.75 8.674 15.904 86.334 1.00 61.95	С
ATOM	7165 C ALA D 491	8.674 15.904 86.334 1.00 61.95	C
ATOM	7166 O ALA D 491	8.204 15.123 87.136 1.00 61.50	0
ATOM	7167 CB ALA D 491	7.429 17.679 85.044 1.00 61.70	C
ATOM	7168 N LYS D 492	9.646 15.491 85.537 1.00 63.32	N
		10.146 14.128 85.511 1.00 64.48	
ATOM	7170 C LYS D 492	10.578 13.747 86.903 1.00 65.18	C O
ATOM	7171 O LYS D 492	10.428 12.584 87.273 1.00 67.28	C
		11.221 13.848 84.463 1.00 63.79	N
	7177 N ALA D 493	11.041 14.629 87.765 1.00 66.09 11.389 14.273 89.140 1.00 66.81	C
	7178 CA ALA D 493	10.128 14.356 90.001 1.00 67.36	c
	7179 C ALA D 493 7180 O ALA D 493	10.063 14.195 91.207 1.00 67.78	Ö
	7181 CB ALA D 493	12.473 15.145 89.721 1.00 65.96	C
	7182 N GLY D 494	9.005 14.625 89.380 1.00 68.06	N
	7183 CA GLY D 494	7.740 14.708 90.043 1.00 69.81	C
	7184 C GLY D 494	7.663 15.827 91.061 1.00 69.63	c
	7185 O GLY D 494	7.480 15.557 92.250 1.00 71.09	Ō
	7186 N LEUD 495	7.765 17.081 90.656 1.00 68.58	N
ATOM		7.591 18.133 91.647 1.00 67.21	C
	7188 C LEU D 495	6.226 18.693 91,258 1.00 67.00	C
	7189 O LEUD 495	5.965 18.674 90.055 1.00 67.42	0
ATOM		8.577 19.265 91.570 1.00 67.41	С

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ATOM	7191 CG LEUD 495	10.064 19.001 91.516 1.00 67.23	С
ATOM	7192 CD1 LEU D 495	10.835 20.279 91.744 1.00 66.57	С
ATOM	7193 CD2 LEU D 495	10.474 17.996 92.580 1.00 68.59	С
ATOM	7194 N THR D 496	5.459 19.174 92.194 1.00 67.01	N
		4.175 19.743 91.803 1.00 68.57	C
ATOM	7196 C THR D 496	4.381 20.804 90.758 1.00 68.94	C
ATOM	7197 O THR D 496	5.466 21.344 90.612 1.00 70.43	0
	7198 CB THR D 496	3.642 20.474 93.043 1.00 69.67	C
		3.559 19.460 94.038 1.00 70.00	0
ATOM	7200 CG2 THR D 496	2.303 21.162 92.843 1.00 72.03	C
ATOM	7201 N LEU D 497	3.354 21.242 90.073 1.00 69.68	N C
	7202 CA LEUD 497	3.459 22.327 89.113 1.00 70.36	C
		3.924 23.570 89.853 1.00 70.71 4.636 24.418 89.326 1.00 71.29	0
ATOM	7204 O LEOD 497	2.089 22.554 88.518 1.00 71.76	C
ATOM	7206 CG LEUD 497	1.898 22.725 87.025 1.00 72.92	č
ATOM	7207 CD1 LEU D 497	1.027 23.981 86.893 1.00 74.10	C
		3.226 22.851 86.288 1.00 73.59	Ċ
		3.526 23.722 91.110 1.00 71.33	N
		3.909 24.874 91.906 1.00 71.87	С
		5.343 24.739 92.364 1.00 70.16	С
	7212 O GLN D 498	6.065 25.726 92.369 1.00 70.91	Ο
		3.011 25.127 93.108 1.00 74.58	С
ATOM	7214 CG GLN D 498	3.668 25.956 94.183 1.00 77.41	C
ATOM	7215 CD GLN D 498	2.776 26.383 95.317 1.00 79.69	С
		2.814 27.551 95.725 1.00 81.49	
		1.968 25.482 95.863 1.00 80.48	
	7218 N GLN D 499		N C
		7.205 23.418 93.118 1.00 66.67	C
ATOM		8.082 23.649 91.889 1.00 65.31 9.207 24.131 91.996 1.00 66.02	O
ATOM ATOM	7221 CB GLN D 499	7.498 22.012 93.605 1.00 67.59	C
	7222 CB GEN D 499	6.331 21.445 94.385 1.00 68.83	Č
	7224 CD GLN D 499	6.815 20.277 95.218 1.00 69.76	Č
	7225 OE1 GLN D 499	7.094 19.197 94.705 1.00 71.19	0
	7226 NE2 GLN D 499	6.905 20.540 96.506 1.00 69.95	N
	7227 N GLN D 500	7.564 23.270 90.726 1.00 62.76	N
	7228 CA GLN D 500	8.296 23.482 89.499 1.00 61.09	С
<b>ATOM</b>	7229 C GLN D 500	8.517 24.994 89.331 1.00 59.09	С
	7230 O GLN D 500	9.691 25,383 89,229 1.00 59.14	0
_	7231 CB GLN D 500	7.540 22.919 88.315 1.00 62.27	C
	7232 CG GLN D 500	7.714 21.442 88.024 1.00 62.80	C
	7233 CD GLN D 500	6.573 20.977 87.142 1.00 63.30	C
	7234 OE1 GLN D 500	6.275 21.531 86.089 1.00 63.54	0 N
ATOM	7235 NE2 GLN D 500	5.917 19.943 87.634 1.00 64.24	N

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ATOM	7281 C ALA D 50	5 13.935 30.831 91.049 1.00 46.17	C
ATOM	7282 O ALA D 50	5 13.935 30.831 91.049 1.00 46.17 5 14.905 31.602 90.909 1.00 47.56	O
ATOM	7283 CB ALA D 5	05 11.568 31.603 90.719 1.00 43.37	. <b>C</b>
		6 13.965 29.871 91.979 1.00 46.90	N
ATOM	7285 CA GLN D 5	06 15.138 29.791 92.857 1.00 46.66	С
		6 16.398 29.604 92.040 1.00 46.13	С
<b>ATOM</b>		6 17.355 30.277 92.381 1.00 46.28	0
$\Delta TOM$	7288 CB GLN D 5	06 15 048 28 771 93 985 1.00 47 09	С
<b>ATOM</b>	7289 CG AGLN D	506 13.658 28.379 94.403 0.50 48.95	С
ATOM	7290 CG BGLN D	506 14.039 29.180 95.048 0.50 47.34	C
<b>ATOM</b>	7291 CD AGLN D	506 13.468 27.457 95.579 0.50 49.86	С
<b>ATOM</b>	7292 CD BGLN D	506 14.421 30.392 95.861 0.50 47.80	С
<b>ATOM</b>	7293 OE1AGLN D	506 14.178 26.464 95.781 0.50 49.50	0
ATOM	7294 OEIBGLND	506 15.594 30.775 95.906 0.50 49.73	0
ATOM	7295 NE2AGLN D	506 12.458 27.779 96.403 0.50 50.31	N
ATOM	7296 NE2BGLN D	506 13.478 31.033 96.532 0.50 46.96	
		7 16.442 28.769 91.020 1.00 47.10	N
	7298 CA LEU D 5	07 17.630 28.522 90.212 1.00 46.22	C
		7 18.072 29.759 89.476 1.00 45.72	C O
ATOM	7300 O LEO D 30	7 19.222 30.170 89.663 1.00 46.37	C
ATOM	7301 CB LEU D 5	07 17.440 27.379 89.226 1.00 47.36 07 17.296 25.982 89.869 1.00 48.45	C
	7302 CG LEU D 3	17.113 24.922 88.794 1.00 48.43	C
		17.113 24.922 88.794 1.00 48.35 607 18.489 25.671 90.748 1.00 48.16	Č
ATOM	7304 CD2 EEU D 2	8 17.175 30.375 88.718 1.00 45.02	N
ATOM	7305 N LLUD 50	08 17.519 31.627 88.020 1.00 43.68	
ATOM		8 17.894 32.743 88.967 1.00 43.09	C
		8 18.818 33.502 88.632 1.00 44.39	O
		08 16.386 32.016 87.074 1.00 43.56	
ATOM	7310 CG LEU D 5	08 16.053 30.912 86.054 1.00 43.99	С
ATOM	7311 CD1 LEU D 5	508 14.857 31.299 85.202 1.00 45.21	С
ATOM	7312 CD2 LEU D 5		C
	7313 N LEUD 50		N
	7314 CA LEU D 5		· C
ATOM	7315 C LEU D 50		. <b>C</b>
ATOM	7316 O LEUD 50		0
	7317 CB LEU D 5		С
	7318 CG LEUD 5		C
	7319 CD1 LEU D 5		C C
ATOM	7320 CD2 LEU D 5		
ATOM	7321 N ILE D 510		N C
ATOM	7322 CA ILE D 51		C
ATOM	7323 C ILE D 510		0
ATOM	7324 O ILE D 510		C
ATOM	7325 CB ILE D 51	0 21.603 31.003 92.070 1.00 41.68	C

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ATOM	7326 CG1 ILE D 510	21.260 30.521 93.473 1.00 42.78	С
<b>ATOM</b>	7327 CG2 ILE D 510	23.086 30.720 91.924 1.00 42.12	С
ATOM	7328 CD1 ILE D 510	20.643 29.129 93.534 1.00 44.12	С
ATOM	7329 N LEUD 511	21.639 33.084 89.512 1.00 39.99	
		22.399 33.641 88.413 1.00 40.71	
ATOM	7331 C LEUD 511	22.747 35.095 88.658 1.00 41.31	C
ATOM	7332 O LEUD 511	23.811 35.561 88.243 1.00 42.30 21.713 33.454 87.078 1.00 41.31	0
ATOM	7333 CB LEU D 511	21.713 33.454 87.078 1.00 41.31	С
		21.424 32.018 86.627 1.00 40.18	
		1 20.905 32.093 85.196 1.00 40.47 1 22.649 31.144 86.777 1.00 38.30	C C
		21.918 35.851 89.341 1.00 41.45	N
		22.208 37.220 89.696 1.00 41.06	
		23.438 37.271 90.603 1.00 41.07	
ATOM	7340 O SER D 512	24 319 38 107 90 419 1 00 42 29	Ö
ATOM	7341 CB SER D 512	24.319 38.107 90.419 1.00 42.29 21.050 37.699 90.583 1.00 42.28	C
ATOM	7342 OG SER D 512	20.792 39.009 90.103 1.00 46.01	0
		23.516 36.375 91.602 1.00 39.13	N
<b>ATOM</b>	7344 CA HIS D 513	24.667 36.326 92.494 1.00 37.67	С
<b>ATOM</b>	7345 C HIS D 513	25.909 35.969 91.689 1.00 37.57	С
<b>ATOM</b>	7346 O HIS D 513	26.965 36.614 91.811 1.00 37.05	0
ATOM	7347 CB HIS D 513	24.431 35.404 93.701 1.00 37.16	С
ATOM	7348 CG AHIS D 513	23.296 36.096 94.421 0.50 37.87 25.455 35.520 94.790 0.50 37.66	C
ATOM	7349 CG BHIS D 513	3 25.455 35.520 94.790 0.50 37.66	C
ATOM	7350 ND1AHIS D 51	3 22.007 35.629 94.434 0.50 38.32	N
		3 26.189 34.437 95.249 0.50 37.48	
ATOM	7352 CD2AHIS D 51	3 23.271 37.255 95.114 0.50 38.08	C
ATOM	7354 CELAMED 51	3 25.857 36.587 95.544 0.50 37.49 31 235 36 403 05 087 0.50 37.64	C C
		3 21.235 36.493 95.087 0.50 37.64 27.001 34.839 96.222 0.50 37.37	
ATOM	7356 NE24HIS D 51	3 21.983 37.457 95.547 0.50 37.37	
	7357 NE2BHIS D 51		N
	7358 N ILED 514	25.801 34.973 90.818 1.00 36.05	N
	7359 CA ILE D 514		C
	7360 C ILED 514	27.359 35.830 89.178 1.00 37.22	С
<b>ATOM</b>	7361 O ILED 514	28.557 36.102 89.102 1.00 37.31	0
<b>ATOM</b>	7362 CB ILE D 514	26.605 33.395 89.163 1.00 38.42	С
ATOM	7363 CG1 ILE D 514	26.580 32.195 90.138 1.00 38.53	С
	7364 CG2 ILE D 514		С
	7365 CD1 ILE D 514		С
	7366 N ARG D 515		N
	7367 CA ARG D 515		С
	7368 C ARGD 515		C
	7369 O ARGD 515		0
AIUM	7370 CB ARG D 515	25.698 38.606 87.335 1.00 40.22	С

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ATOM	7416 CE LYS D 520	31.685 43.833 93.425 1.00 55.68	С
ATOM	7417 NZ LYS D 520	32.165 45.060 94.170 1.00 57.32	N
	7418 N GLY D 521		N
		36.244 38.630 90.408 1.00 45.07	С
ATOM	7420 C GLY D 521	37.027 39.378 89.335 1.00 45.97	С
<b>ATOM</b>	7421 O GLY D 521	38.255 39.361 89.546 1.00 46.47	0
		36.453 39.964 88.263 1.00 45.24	N
		37.330 40.608 87.313 1.00 46.17	С
	7424 C MET D 522		С
	7425 O MET D 522		0
		36.883 41.251 86.040 1.00 46.68	С
		35.743 40.908 85.172 1.00 47.01	С
		36.052 39.568 84.026 1.00 47.12	S
		37.801 39.701 83.767 1.00 45.10	С
		37.206 42.542 88.805 1.00 48.67	N
		37.853 43.687 89.453 1.00 49.92	C
		39.105 43.238 90.179 1.00 46.61	C
	7433 O GLUD 523		0
		36.858, 44.389, 90.334, 1.00, 56.37	C
		36.040 45.451 89.644 1.00 63.92	
		36.859 46.494 88.902 1.00 68.65	
		38.084 46.628 89.154 1.00 70.98	0
		36.213 47.184 88.057 1.00 71.61	O N
		39.085 42.164 90.931 1.00 44.00 40.206 41.623 91.631 1.00 42.73	C
	7440 CA HIS D 524 7441 C HIS D 524		c
		42.462 41.370 90.874 1.00 43.70	0
		39.722 40.452 92.478 1.00 42.39	C
		40.786 39.709 93.209 1.00 42.67	
		41.535 38.688 92.672 1.00 43.20	N
ATOM	7446 CD2 HIS D 524	41.257 39.812 94.461 1.00 43.18	Ċ
	7447 CE1 HIS D 524	42.409 38.233 93.536 1.00 42.46	Č
	7448 NE2 HIS D 524	42.260 38.896 94.651 1.00 42.25	N
	7449 N LEU D 525	40.964 40.309 89.687 1.00 45.58	N
	7450 CA LEUD 525	41.967 39.726 88.807 1.00 47.55	С
	7451 C LEUD 525	42.777 40.855 88.195 1.00 50.31	С
	7452 O LEUD 525	43.968 40.797 87.964 1.00 50.79	0
	7453 CB LEUD 525	41.392 38.854 87.698 1.00 46.07	С
ATOM	7454 CG LEUD 525	42.393 38.273 86.703 1.00 44.46	С
<b>ATOM</b>	7455 CD1 LEU D 525	43.376 37.351 87.404 1.00 43.93	С
<b>ATOM</b>	7456 CD2 LEU D 525	41.671 37.541 85.593 1.00 43.69	С
ATOM	7457 N TYR D 526	42.062 41.918 87.912 1.00 53.91	N
ATOM	7458 CA TYR D 526	42.581 43.132 87.344 1.00 57.32	С
ATOM	7459 C TYR D 526	43.546 43.787 88.302 1.00 58.27	С
ATOM	7460 O TYR D 526	44.621 44.138 87.853 1.00 59.84	Ο

51.263 43.253 89.316 1.00 85.75 ATOM 7508 N ASN D 532 N ATOM 7509 CA ASN D 532 52.214 42.377 88.674 1.00 87.67 C 52.414 41.123 89.498 1.00 86.83 C ATOM 7510 C ASN D 532 ATOM 7511 O ASN D 532 53,503 40,824 89,973 1,00 88,13 0 ATOM 7512 CB ASN D 532 53,540 43,116 88,492 1.00 91,44 C ATOM 7513 CG ASN D 532 53.396 44.210 87.448 1.00 95.11 C ATOM 7514 OD1 ASN D 532 52.743 43.976 86.413 1.00 96.83 0 53.984 45.380 87.725 1.00 96.52 ATOM 7515 ND2 ASN D 532 N ATOM 7516 N VAL D 533 51.372 40.355 89.738 1.00 85.40 N ATOM 7517 CA VAL D 533 51.384 39.134 90.532 1.00 83.94 C ATOM 7518 C VAL D 533 50.924 37.951 89.675 1.00 83.81 C ATOM 7519 O VAL D 533 51.168 36.756 89.856 1.00 84.37 O ATOM 7520 CB VAL D 533 50.376 39.287 91.689 1.00 83.16 C ATOM 7521 CG1 VAL D 533 50.469 38.081 92.594 1.00 83.74 C ATOM 7522 CG2 VAL D 533 50.551 40.567 92.473 1.00 82.60 C ATOM 7523 N VAL D 534 50.172 38.318 88.640 1.00 82.67 N ATOM 7524 CA VAL D 534 49.598 37.434 87.666 1.00 81.37 C ATOM 7525 C VAL D 534 50.520 37.295 86.464 1.00 80.71 ATOM 7526 O VAL D 534 50.947 38.270 85.846 1.00 79.76 O ATOM 7527 CB VAL D 534 48.261 38.000 87.145 1.00 81.77 C ATOM 7528 CG1 VAL D 534 47.647 37.281 85.967 1.00 81.40 C ATOM 7529 CG2 VAL D 534 47,263 38,076 88,282 1.00 82,95 C 50.788 36.051 86.118 1.00 80.27 ATOM 7530 N PRO D 535 N 51.570 35.696 84.968 1.00 80.35 ATOM 7531 CA PRO D 535 C ATOM 7532 C PRO D 535 50.835 36.148 83.705 1.00 81.79 ATOM 7533 O PRO D 535 49.647 36.476 83.597 1.00 81.91 0 ATOM 7534 CB PRO D 535 51,709 34,172 84,941 1.00 79.80 C 51.017 33.727 86.177 1.00 79.58 ATOM 7535 CG PRO D 535 C C ATOM 7536 CD PRO D 535 50.276 34.869 86.810 1.00 80.22 51.630 36.118 82.638 1.00 83.19 ATOM 7537 N LEU D 536 N ATOM 7538 CA LEU D 536 51.243 36.490 81.306 1.00 83.84 C ATOM 7539 C LEU D 536 50.532 35.437 80.481 1.00 83.18 C ATOM 7540 O LEUD 536 50.977 35.207 79.347 1.00 85.15 0 49.468 34.835 80.990 1.00 80.74 ATOM 7545 N TYR D 537 N ATOM 7546 CA TYR D 537 48.744 33.854 80.189 1.00 77.68 C ATOM 7547 C TYR D 537 47.933 34.693 79.202 1.00 75.48 C ATOM 7548 O TYR D 537 47.192 35.577 79.597 1.00 74.48 0 ATOM 7549 CB TYR D 537 47.865 32.974 81.033 1.00 78.11 C ATOM 7550 CG TYR D 537 48.632 32.199 82.075 1.00 78.38 C 49.603 31.297 81.691 1.00 79.18 C ATOM 7551 CD1 TYR D 537 C ATOM 7552 CD2 TYR D 537 48.385 32.348 83.424 1.00 78.50 ATOM 7553 CE1 TYR D 537 50.311 30.557 82.619 1.00 79.58 C C ATOM 7554 CE2 TYR D 537 49.095 31.609 84.339 1.00 78.93 50.052 30.717 83.956 1.00 79.10 C ATOM 7555 CZ TYR D 537 ATOM 7556 OH TYR D 537 50.760 29.987 84.870 1.00 79.09 0

wo	98/5681	12	<b>,</b>	PCT/
			777/371	
ATOM	7557	N ASP D 538	48.135 34.396 77.933 1.00 73.43	N
			47.485 35.097 76.862 1.00 71.14	С
		C ASP D 538		С
		O ASP D 538		Ο
			48.112 34.546 75.573 1.00 76.06	С
			49.333 35.379 75.241 1.00 80.52	С
			49.297 36.609 75.511 1.00 83.41	0
ATOM	7564	OD2 ASP D 538	50.312 34.803 74.721 1.00 83.00	Ο
		N LEU D 539		N
ATOM	7566	CA LEU D 539	43.949 33.698 76.631 1.00 56.68	С
ATOM	7567	C LEU D 539	43.198 34.354 77.772 1.00 55.11	С
		O LEU D 539		O
			43.587 32.246 76.374 1.00 53.99	С
ATOM	7570	CG LEUD 539	42.176 31.839 76.024 1.00 51.86	C
			41.595 32.693 74.914 1.00 51.90	C
			42.139 30.375 75.652 1.00 51.00	C
		N LEU D 540		N
			43.192 34.833 80.182 1.00 51.65	C
		C LEU D 540		С
		O LEUD 540		0
			43.870 34.292 81.437 1.00 49.81	C C
			43.283 34.798 82.757 1.00 49.22	C
		<del>-</del>	41.996 34.063 83.099 1.00 48.02	C
		CD2 LEU D 540	44.251 34.717 83.918 1.00 47.83 44.395 36.924 79.627 1.00 52.89	N
		N LEUD 541	44.461 38.378 79.526 1.00 54.36	C
		C LEU D 541		c
			42.957 39.961 78.564 1.00 55.08	Ö
ATOM	7585	CR I FII D 541	45.882 38.908 79.365 1.00 56.82	Č
			46.746 38.458 80.562 1.00 59.61	Č
			48.213 38.814 80.410 1.00 60.75	
			46.199 38.946 81.895 1.00 59.95	
ATOM		N GLU D 542	43,283 38.046 77.436 1.00 52.05	N
ATOM		CA GLUD 542	42.359 38.419 76.378 1.00 52.01	С
ATOM		C GLU D 542	40.962 38.558 76.964 1.00 51.81	С
ATOM		O GLU D 542	40.343 39.603 76.763 1.00 52.56	Ο
ATOM		CB GLU D 542	42.374 37.375 75.286 1.00 52.93	С
<b>ATOM</b>	7594	CG GLUD 542	41.504 37.629 74.073 1.00 54.03	С
<b>ATOM</b>	7595	CD GLUD 542	41.813 36.554 73.045 1.00 55.61	С
<b>ATOM</b>	7596	OE1 GLU D 542	43.002 36.118 73.040 1.00 56.51	0
ATOM	7597	OE2 GLU D 542	40,862 36.198 72.325 1.00 55.79	0
$\boldsymbol{ATOM}$	7598	N MET D 543	40.460 37.558 77.678 1.00 50.53	N
ATOM		CA MET D 543	39.128 37.617 78.249 1.00 48.98	C
ATOM	7600	C MET D 543	39.009 38.734 79.250 1.00 49.90	C
<b>ATOM</b>	7601	O MET D 543	37.965 39.392 79.390 1.00 50.42	Ο

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ATOM		CB MET D 543	38.864 36.247 78.858 1.00 49.15	C
ATOM		CG MET D 543	39.038 35.161 77.798 1.00 49.35	C
ATOM		SD MET D 543	37.661 35.157 76.652 1.00 49.50	S C
ATOM		CE MET D 543	38.446 35.461 75.101 1.00 50.34	N
ATOM		N LEUD 544 CA LEUD 544	40.084 38.981 80.006 1.00 50.40 40.087 40.046 81.006 1.00 49.64	C
ATOM ATOM		C LEU D 544	40.020 41.371 80.274 1.00 51.52	C
ATOM		O LEU D 544	39.243 42.187 80.742 1.00 51.84	0
ATOM		CB LEU D 544	41.266 39.974 81.932 1.00 47.56	C
ATOM		CG LEU D 544	41.587 41.124 82.855 1.00 46.86	č
ATOM		CD1 LEU D 544	40.531 41.407 83.893 1.00 47.36	Č
ATOM		CD2 LEU D 544	42.858 40.857 83.633 1.00 46.52	č
ATOM		N ASP D 545	40.742 41.598 79.188 1.00 54.73	N
ATOM		CA ASP D 545	40.657 42.868 78.490 1.00 58.31	С
<b>ATOM</b>	7616	C ASP D 545	39.293 43.125 77.904 1.00 58.22	С
<b>ATOM</b>		O ASP D 545	38.857 44.265 77.953 1.00 58.37	0
ATOM		CB ASP D 545	41.660 43.039 77.359 1.00 63.15	С
ATOM		CG ASP D 545	43.086 43.066 77.858 1.00 68.13	С
ATOM		OD1 ASP D 545	43.347 43.145 79.089 1.00 71.17	0
ATOM		OD2 ASP D 545	44.001 43.000 76.998 1.00 70.50	.0
ATOM		N ALAD 546	38.569 42.144 77.404 1.00 59.16	N
ATOM		CA ALA D 546	37.246 42.333 76.848 1.00 59.75	C
ATOM		C ALA D 546 O ALA D 546	36.414 43.173 77.792 1.00 61.95 35.707 44.069 77.382 1.00 62.80	C O
ATOM ATOM		CB ALA D 546	36.535 41.025 76.647 1.00 59.19	C
ATOM		N HIS D 547	36.464 42.895 79.070 1.00 65.29	N
ATOM		CA HIS D 547	35.762 43.580 80.115 1.00 68.19	Ĉ
ATOM		C HIS D 547	36.237 44.968 80.398 1.00 72.31	c
ATOM		O HIS D 547	35.418 45.857 80.570 1.00 74.57	0
ATOM		CB HIS D 547	35.976 42.771 81.426 1.00 66.78	С
<b>ATOM</b>	7632	CG HIS D 547	34.987 41.661 81.222 1.00 65.39	С
		ND1 HIS D 547	33.769 41.664 81.821 1.00 65.32	N
		CD2 HIS D 547	35.060 40.566 80.449 1.00 65.37	С
		CE1 HIS D 547		С
		NE2 HIS D 547	33.870 39.902 80.597 1.00 65.28	N
		N ARG D 548	37.527 45.178 80.481 1.00 77.80	N
		CA ARG D 548	38.011 46.541 80.764 1.00 83.04	C
		C ARGD 548	37.660 47.467 79.610 1.00 83.91	С
		O ARG D 548 CB ARG D 548	37.280 46.990 78.509 1.00 84.82 39.503 46.486 81.078 1.00 86.73	O C
		CG ARG D 548	40.043 45.244 81.771 1.00 89.93	C
		CD ARG D 548		c
		NE ARG D 548		N
		CZ ARG D 548		Ĉ
		NH1 ARG D 548		N
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ATOM 7647 NH2 ARG D 548	•	N
TER 7648 ARG D 548		
HETATM 7649 C1 EST D 600	40.094 29.783 88.544 1.00 35.42	С
HETATM 7650 C2 EST D 600	39.609 28.605 87.970 1.00 37.10	С
HETATM 7651 C3 EST D 600	38.284 28.306 88.112 1.00 38.08	С
HETATM 7652 O3 EST D 600	37.791 27.149 87.568 1.00 39.71	O
HETATM 7653 C4 EST D 600	37.364 29.111 88.801 1.00 37.36	С
HETATM 7654 C5 EST D 600		
HETATM 7655 C6 EST D 600	36.954 31.006 90.323 1.00 36.00	
HETATM 7656 C7 EST D 600	37.659 32.135 91.080 1.00 35.08	
HETATM 7657 C8 EST D 600		
	39.773 31.877 89.830 1.00 34.03	
	39,229 30.633 89.231 1.00 34.86	
	40.843 32.524 88.969 1.00 34.70	
HETATM 7661 C12 EST D 600	41.482 33.712 89.730 1.00 34.68	
HETATM 7662 C13 EST D 600		
HETATM 7663 C14 EST D 600	39.274 33.993 90.916 1.00 34.39	С
	38.441 35.195 91.345 1.00 35.06	
HETATM 7665 C16 EST D 600	39.571 36.111 91.977 1.00 34.28	С
	40.746 35.820 91.048 1.00 34.55	
HETATM 7667 O17 EST D 600	41.355 36.988 90.563 1.00 34.28	
	39.825 35.299 88.774 1.00 32.87	C
	66.664 39.609 24.082 1.00 90.13	N
	66.219 40.728 24.958 1.00 89.20	С
ATOM 7671 C SER E 305	67.314 41.258 25.867 1.00 88.52	C
ATOM 7672 O SER E 305	67.943 40.498 26.603 1.00 88.14	0
ATOM 7673 CB SER E 305	65.012 40.240 25.772 1.00 89.12	C
	64.518 41.250 26.629 1.00 89.17	
ATOM 7675 N LEUE 306	67.515 42.577 25.872 1.00 88.09	
	68.491 43.194 26.776 1.00 87.38	С
ATOM 7677 C LEUE 306	68.152 42.634 28.161 1.00 86.17	C
ATOM 7678 O LEUE 306	68.964.42.011 28.838 1.00 86.28	0 ,
ATOM 7679 CB LEUE 306	68.412 44.719 26.769 1.00 87.54	C
ATOM 7683 N ALA E 307	66.897 42.808 28.562 1.00 84.21	N
ATOM 7684 CA ALA E 307	66.416 42.301 29.824 1.00 82.98	С
ATOM 7685 C ALA E 307	67.160 41.033 30.203 1.00 81.72	C
ATOM 7686 O ALA E 307	67.884 41.044 31.195 1.00 81.98	0
ATOM 7687 CB ALA E 307	64.934 41.958 29.746 1.00 83.87	C
ATOM 7688 N LEUE 308	67.010 39.986 29.409 1.00 80.54	N
ATOM 7689 CA LEU E 308	67.654 38.722 29.711 1.00 80.61	С
ATOM 7690 C LEUE 308	69.161 38.703 29.707 1.00 81.30	C
ATOM 7691 O LEUE 308	69.724 37.659 30.049 1.00 82.75	0
ATOM 7692 CB LEUE 308	67.085 37.650 28.782 1.00 80.17	C C
ATOM 7693 CG LEUE 308	65.577 37.475 28.851 1.00 81.19	C
ATOM 7694 CD1 LEU E 308	65.154 36.148 28.222 1.00 81.69	C

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7695	<b>CD2 LEU E 308</b>	65.053 37.544 30.286 1.00 81.62	С
7696	N SER E 309	69.908 39,736 29.387 1.00 80.88	N
7697	CA SER E 309	71.347 39.770 29.359 1.00 80.22	C
7698	C SER E 309	71.999 40.597 30.445 1.00 78.84	С
7699	O SER E 309	73.155 40.377 30.811 1.00 79.47	0
7700	CB SER E 309	71.753 40.479 28.045 1.00 81.59	С
7701	OG SER E 309	70.952 39.844 27.041 1.00 84.79	0
7702	N LEU E 310	71.283 41.600 30.940 1.00 77.00	N
7703	CA LEUE 310	71.887 42.438 31.972 1.00 74.38	С
7704	C LEUE310	72.143 41.592 33.215 1.00 72.92	С
7705	O LEUE 310	71.526 40.578 33.479 1.00 72.38	0
7706	CB LEUE 310	71.076 43.676 32.277 1.00 73.94	С
		70.244 44.241 31.131 1.00 73.26	С
		68.782 44.089 31.487 1.00 73.44	С
7709	CD2 LEU E 310	70.608 45.687 30.897 1.00 74.10	С
		73.126 42.065 33.953 1.00 71.49	N
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7739	N METE 315	70.760 45,697 35.720 1.00 64.89	N
	7696 7697 7698 7699 7700 7701 7702 7703 7704 7705 7706 7707 7708 7709 7710 7711 7712 7713 7714 7715 7716 7717 7718 7719 7720 7721 7722 7723 7724 7725 7726 7727 7728 7729 7730 7731 7732 7733 7734 7735 7736 7737 7738	7696 N SER E 309 7697 CA SER E 309 7698 C SER E 309 7699 O SER E 309 7700 CB SER E 309 7701 OG SER E 309 7702 N LEU E 310 7703 CA LEU E 310 7704 C LEU E 310 7706 CB LEU E 310 7706 CB LEU E 310 7707 CG LEU E 310 7708 CD1 LEU E 310 7709 CD2 LEU E 310 7710 N THR E 311 7711 CA THR E 311 7712 C THR E 311 7713 O THR E 311 7714 CB THR E 311 7715 OG1 THR E 311 7716 CG2 THR E 311 7717 N ALA E 312 7718 CA ALA E 312 7719 C ALA E 312 7719 C ALA E 312 7719 C ALA E 312 7720 O ALA E 312 7721 CB ALA E 312 7721 CB ALA E 312 7722 N ASP E 313 7723 CA ASP E 313 7724 C ASP E 313	7695 CD2 LEU E 308 7696 N SER E 309 7697 CA SER E 309 7698 C SER E 309 7699 O SER E 309 7700 CB SER E 309 7701 OG SER E 309 7701 OG SER E 309 7702 N LEU E 310 7704 C LEU E 310 7705 O LEU E 310 7706 CB LEU E 310 7707 CG LEU E 310 7707 CG LEU E 310 7708 CD1 LEU E 310 7709 CD2 LEU E 310 7709 CD2 LEU E 310 7710 N THR E 311 7711 CA THR E 311 7711 CA THR E 311 7712 C THR E 311 7714 CB THR E 311 7715 OG1 THR E 311 7716 CG2 THR E 311 7717 N ALA E 312 7719 C ALA E 312 7719 C ALA E 312 7720 O ALA E 312 7720 O ALA E 312 7721 CB ALA E 312 7722 O ASP E 313 7725 CA ASP E 313 7726 CB ASP E 313 7727 CG ASP E 313 7728 OD1 ASP E 313 7729 OD2 ASP E 313 7730 N GLN E 314 7731 CG GLN E 314 7733 C GLN E 314 7734 CB GLN E 314 7735 CG GLN E 314 7736 CD GLN E 314 7737 OEI GLN E 314 7738 NE2 GLN E 314 7748 NE2 GLN E 314 775.561 44.5682 31.887 1.00 77.18

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ATOM	7740 CA MET E 315	69.321 45.727 35.900 1.00 61.52	С
	7741 C MET E 315		c
		68.232 47.738 36.694 1.00 59.18	0
<b>ATOM</b>	7743 CB MET E 315	68.866 44.369 36.399 1.00 61.20	С
<b>ATOM</b>	7744 CG MET E 315	67.374 44.157 36.557 1.00 61.73	С
ATOM	7745 SD MET E 315	66.545 43.770 34.975 1.00 60.72	S
ATOM	7746 CE MET E 315	65.521 45.250 34.944 1.00 61.58	С
ATOM			N
		69.334 47.693 39.160 1.00 58.51	С
		69.568 49.109 38.668 1.00 59.26	C
ATOM		68.757 49.996 38.917 1.00 60.99	0
ATOM		70.182 47.522 40.426 1.00 57.64 69.926 48.654 41.412 1.00 56.70	C
		69.871 46.177 41.069 1.00 57.96	C C
		70.665 49.373 38.003 1.00 59.51	N
ATOM		70.944 50.739 37.560 1.00 60.83	C
		70.009 51.159 36.456 1.00 59.74	c
		69.545 52.304 36.418 1.00 60.86	Ö
		72.391 50.810 37.057 1.00 62.92	C
		72.768 49.429 36.981 1.00 66.28	Ο
		69.718 50.225 35.560 1.00 57.32	N
<b>ATOM</b>	7761 CA ALA E 318	68.783 50.552 34.489 1.00 55.79	C
ATOM	7762 C ALA E 318	67.476 51.078 35.083 1.00 55.92	С
ATOM		66.890 52.070 34.648 1.00 55.88	0
		68.486 49.293 33.718 1.00 55.78	C
	7765 N LEUE 319		N
		65.771 50.688 36.813 1.00 52.78	C
ATOM		65.972 51.959 37.583 1.00 54.13	C
ATOM		65.170 52.873 37.500 1.00 54.67 65.441 49.546 37.767 1.00 50.55	O C
		64.947 48.274 37.072 1.00 49.71	C
	7771 CD1 LEU E 319	64.666 47.218 38.123 1.00 48.77	C
	7772 CD2 LEU E 319		Č
	7773 N LEUE 320	67.090 52.082 38.278 1.00 56.12	N
	7774 CA LEUE 320	67.366 53.288 39.055 1.00 58.13	C
	7775 C LEUE 320	67.378 54.490 38.144 1.00 60.62	С
<b>ATOM</b>	7776 O LEUE 320	67.002 55.584 38.522 1.00 62.27	0
<b>ATOM</b>	7777 CB LEUE 320	68.697 53.147 39.799 1.00 57.11	С
ATOM	7778 CG LEUE 320	68.449 52.587 41.195 1.00 56.24	С
	7779 CD1 LEU E 320	69.771 52.365 41.887 1.00 57.34	C
	7780 CD2 LEU E 320	67.526 53.555 41.901 1.00 55.80	С
	7781 N ASP E 321	67.814 54.306 36.919 1.00 63.78	N
	7782 CA ASP E 321	67.844 55.362 35.948 1.00 67.74	C
	7783 C ASP E 321	66.504 55.768 35.388 1.00 66.51	С
ATUM	7784 O ASP E 321	66.284 56.942 35.112 1.00 68.09	0

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<b>ATOM</b>	7785	CB ASP E 321	68.660 54.866 34.732 1.00 73.25	С
<b>ATOM</b>	7786	CG ASP E 321	70.007 55.573 34.820 1.00 78.83	С
<b>ATOM</b>	7787	OD1 ASP E 321	70.229 56.287 35.842 1.00 81.54	0
<b>ATOM</b>	7788	OD2 ASP E 321	70.810 55.390 33.871 1.00 81.74	0
<b>ATOM</b>	7789	N ALA E 322	65.596 54.825 35.185 1.00 63.63	N
<b>ATOM</b>	7790	CA ALAE 322	64.310 55.135 34.587 1.00 60.60	С
<b>ATOM</b>	7791	C ALA E 322	63.429 55.954 35.499 1.00 59.85	С
<b>ATOM</b>	7792	O ALA E 322	62.408 56.514 35.072 1.00 59.85	0
<b>ATOM</b>	7793	CB ALAE 322	63.663 53.798 34.246 1.00 60.27	С
<b>ATOM</b>	7794	N GLU E 323	63.770 56.023 36.786 1.00 58.01	N
<b>ATOM</b>	7795	CA GLUE 323	62.919 56.750 37.730 1.00 55.97	С
<b>ATOM</b>	7796	C GLU E 323	62.490 58.058 37.151 1.00 55.08	С
<b>ATOM</b>	7797	O GLU E 323	63.247 58.786 36.523 1.00 57.54	Ο
<b>ATOM</b>	7798	CB GLUE 323	63.694 56.817 39.039 1.00 55.76	С
<b>ATOM</b>	7799	CG GLUE 323	63.544 55.500 39.811 1.00 55.81	С
<b>ATOM</b>	7800	CD GLUE 323	62.152 55.434 40.397 1.00 56.70	С
<b>ATOM</b>	7801	OE1 GLU E 323	61.776 56.308 41.211 1.00 57.38	Ο
ATOM	7802	<b>OE2 GLU E 323</b>	61.381 54.527 40.053 1.00 57.03	Ο
ATOM	7803	N PRO E 324	61.243 58.415 37.306 1.00 54.39	N
ATOM	7804	CA PROE 324	60.676 59.671 36.823 1.00 53.99	С
ATOM	7805	C PRO E 324	61.006 60.793 37.785 1.00 53.72	С
ATOM	7806	O PRO E 324		0
ATOM	7807	CB PROE 324	59.153 59.457 36.810 1.00 53.22	С
		CG PROE 324	59.024 58.476 37.934 1.00 53.17	C
		CD PROE 324	60.264 57.627 38.049 1.00 53.88	С
		N PRO E 325	60.760 62.008 37.397 1.00 53.96	N
		CA PRO E 325	60.981 63.188 38.208 1.00 55.99	С
		C PRO E 325	59.956 63.279 39.316 1.00 57.54	С
		O PRO E 325		О
		CB PROE 325		С
			59.841 63.787 36.229 1.00 55.04	C -
		CD PROE 325	60.207 62.331 36.081 1.00 54.93	С
		N ILE E 326	60.110 64.010 40.390 1.00 59.40	N
ATOM		CA ILE E 326	59.047 64.094 41.405 1.00 62.16	С
		C ILE E 326	58.231 65.358 41.070 1.00 60.95	C
		O ILE E 326	58.865 66.421 40.958 1.00 61.11	0
		CB ILE E 326	59.425 64.267 42.892 1.00 64.57	C
		CG1 ILE E 326	60.372 65.455 43.142 1.00 67.03	C
		CG2 ILE E 326	60.016 62.999 43.511 1.00 64.53	C
		CD1 ILE E 326	61.627 65.591 42.290 1.00 69.10	С
ATOM		N LEUE 327	56.928 65.259 40.897 1.00 59.14	N
ATOM		CA LEUE 327	56.176 66.473 40.595 1.00 57.57	С
ATOM		C LEUE 327	55.911 67.247 41.875 1.00 58.33	C
		O LEU E 327	56.166 66.834 42.999 1.00 57.32	0
ATOM	7829	CB LEUE 327	54.907 66.051 39.874 1.00 56.25	С

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ATOM	7830 CG LEUE 327	/	С
ATOM	7831 CD1 LEU E 327	53.826 65.144 37.802 1.00 55.31	С
ATOM	7832 CD2 LEU E 327	56.305 65.426 37.874 1.00 55.58	С
ATOM	7833 N TYR E 328	55.396 68.458 41.735 1.00 60.55	N
ATOM	7834 CA TYR E 328	55.008 69.326 42.832 1.00 62.06	С
ATOM	7835 C TYR E 328	53.498 69.533 42.642 1.00 63.12	C
ATOM	7836 O TYR E 328	53.050 69.583 41.495 1.00 62.44	Ο
ATOM	7837 CB TYR E 328	55.674 70.709 42.851 1.00 62.29	С
ATOM	7838 CG TYR E 328	57.079 70.585 43.383 1.00 62.82	С
<b>ATOM</b>	7839 CD1 TYR E 328	57.303 70.581 44.747 1.00 63.59	С
<b>ATOM</b>	7840 CD2 TYR E 328	58.168 70.444 42.546 1.00 63.07	С
<b>ATOM</b>	7841 CE1 TYR E 328	58.587 70.447 45.235 1.00 64.17	С
<b>ATOM</b>	7842 CE2 TYR E 328	59.455 70.304 43.031 1.00 63.49	С
<b>ATOM</b>	7843 CZ TYR E 328	59.657 70.302 44.386 1.00 64.13	С
ATOM	7844 OH TYR E 328	60.928 70.165 44.899 1.00 65.08	О
<b>ATOM</b>	7845 N SER E 329	52.766 69.635 43.728 1.00 65.10	N
ATOM	7846 CA SER E 329	51.337 69.839 43.584 1.00 67.67	С
ATOM	7847 C SER E 329	51.090 71.276 43.149 1.00 70.67	C
ATOM	7848 O SER E 329	51.825 72.164 43.562 1.00 70.24	O
<b>ATOM</b>	7849 CB SER E 329	50.621 69.568 44.903 1.00 66.71	С
ATOM	7850 OG SER E 329	49.353 70.169 44.764 1.00 67.28	Ο
<b>ATOM</b>	7851 N GLUE 330	50.068 71.489 42.340 1.00 75.59	N
<b>ATOM</b>	7852 CA GLUE 330	49.667 72.797 41.847 1.00 79.74	С
<b>ATOM</b>	7853 C GLUE 330	49.227 73.680 43.009 1.00 80.39	С
<b>ATOM</b>	7854 O GLUE 330	48.555 73.276 43.957 1.00 80.63	О
<b>ATOM</b>	7855 CB GLUE 330	48.524 72.672 40.843 1.00 83.66	С
<b>ATOM</b>	7856 CG GLUE 330	47.189 73.282 41.204 1.00 88.63	С
ATOM	7857 CD GLUE 330	46.072 72.327 41.592 1.00 91.97	С
<b>ATOM</b>	7858 OE1 GLU E 330	45.391 71.767 40.683 1.00 93.20	0
<b>ATOM</b>	7859 OE2 GLU E 330	45.821 72.110 42.814 1.00 93.64	0
<b>ATOM</b>	7860 N PHE E 337	40.305 73.124 51.688 1.00 85.22	N
<b>ATOM</b>	7861 CA PHE E 337	40.117 71.718 51:376 1.00 84.72	С
ATOM	7862 C PHE E 337	38.650 71.308 51.477 1.00 83.52	С
ATOM	7863 O PHE E 337	38.042 71.506 52.526 1.00 84.39	0
ATOM	7864 CB PHE E 337	40.874 70.727 52.265 1.00 85.39	С
<b>ATOM</b>	7865 CG PHE E 337	42.298 70.544 51.823 1.00 86.55	С
<b>ATOM</b>	7866 CD1 PHE E 337	42.658 70.658 50.496 1.00 87.08	С
ATOM	7867 CD2 PHE E 337	43.280 70.276 52.755 1.00 87.08	С
ATOM	7868 CE1 PHE E 337	43.966 70.504 50.112 1.00 87.85	С
ATOM	7869 CE2 PHE E 337	44.588 70.119 52.384 1.00 87.59	С
ATOM	7870 CZ PHE E 337	44.932 70.231 51.053 1.00 88.06	С
ATOM	7871 N SER E 338	38.134 70.743 50.400 1.00 80.45	N
ATOM	7872 CA SER E 338	36.748 70.299 50.424 1.00 77.39	С
ATOM	7873 C SER E 338	36.773 69.014 49.635 1.00 75.91	C
<b>ATOM</b>	7874 O SER E 338	37.700 68.892 48.837 1.00 76.77	Ο

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			285/371	
ATOM	7920	O LEUE 345	46.007 66.515 42.626 1.00 49.85	Ο
ATOM		CB LEUE 345	45.081 68.394 45.131 1.00 53.85	С
ATOM		CG LEU E 345	44.953 69.833 45.603 1.00 56.56	С
ATOM	7923	CD1 LEU E 345	44.136 69.811 46.891 1.00 57.16	C
ATOM	7924	CD2 LEU E 345	46.313 70.472 45.781 1.00 56.83	C
ATOM	7925	N LEUE 346	44.571 65.814 44.258 1.00 49.14	N
ATOM	7926	CA LEU E 346	44.986 64.418 44.177 1.00 47.49	С
ATOM		C LEU E 346	44.896 63.900 42.760 1.00 46.79	С
ATOM		O LEU E 346	45.813 63.355 42.149 1.00 45.83	0
ATOM		CB LEUE 346	44.110 63.680 45.186 1.00 47.01	С
ATOM		CG LEU E 346	44.533 63.926 46.634 1.00 47.91	C
ATOM		CD1 LEU E 346	43.936 62.861 47.554 1.00 47.78	C
ATOM		CD2 LEU E 346	46.047 63.950 46.838 1.00 47.51	C
ATOM		N THR E 347	43.722 64.101 42.185 1.00 45.98	N
ATOM		CA THR E 347	43.387 63.697 40.825 1.00 45.47	C
ATOM		C THR E 347	44.236 64.394 39.803 1.00 46.07	C O
ATOM	7936		44.710 63.770 38.859 1.00 46.31 41.876 63.928 40.726 1.00 45.77	C
ATOM		CB THR E 347	41.285 62.634 40.726 1.00 45.77	C
ATOM ATOM		OG1 THR E 347 CG2 THR E 347	41.473 64.979 39.747 1.00 45.14	C
ATOM		N ASNE 348	44.512 65.679 39.952 1.00 47.18	N
ATOM	-	CA ASN E 348	45.376 66.434 39.055 1.00 47.33	C
ATOM		C ASN E 348	46.804 65.869 39.095 1.00 45.16	c
ATOM		O ASN E 348	47.477 65.591 38.118 1.00 44.24	Ö
ATOM		CB ASN E 348	45,386 67.899 39.504 1.00 50.18	C
ATOM		CG ASN E 348	46.348 68.766 38.697 1.00 54.12	С
ATOM		OD1 ASN E 348	47,532 69,034 39,065 1,00 54,75	C
ATOM		ND2 ASN E 348	45.771 69.187 37.550 1.00 54.87	N
<b>ATOM</b>	7948	N LEU E 349	47.335 65.683 40.286 1.00 43.41	N
<b>ATOM</b>	7949	CA LEUE 349	48.674 65.173 40.501 1.00 42.15	С
ATOM		C LEU E 349	48.756 63.811 39.856 1.00 42.03	С
		O LEU E 349	49.757 63.555 39.179 1.00 43.04	· O.
		CB LEU E 349	48.968 65.152 42.004 1.00 42.95	C
		CG LEU E 349	50.340 64.653 42.411 1.00 43.25	C
		CD1 LEU E 349	51.417 65.586 41.855 1.00 43.86	C
		CD2 LEU E 349	50.481 64.509 43.905 1.00 43.16	C
		N ALAE 350	47.759 62.935 40.017 1.00 40.82	N
ATOM		CA ALAE 350	47.776 61.615 39.414 1.00 39.79	C
ATOM		C ALAE350	47.854 61.751 37.900 1.00 41.20	C O
ATOM		O ALA E 350	48.729 61.187 37.235 1.00 41.18	C
ATOM		CB ALA E 350	46.545 60.810 39.745 1.00 39.02 46.952 62.556 37.331 1.00 42.05	N
ATOM		N ASP E 351 CA ASP E 351	46.960 62.747 35.894 1.00 43.55	C
ATOM		C ASP E 351	48.325 63.146 35.367 1.00 44.64	C
ATOM ATOM	7964		48.749 62.760 34.258 1.00 45.95	Ö
AT OM	1704	O MOLE 331	70,177 02,100 37.230 1.00 73.23	•

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ΔΤΩΜ	7065 CR ASP F 351	45.892 63.754 35.534 1.00 45.99	С
ATOM	7966 CG ASP F 351	45.849 63.920 34.033 1.00 49.35	Č
		45.353 63.008 33.355 1.00 51.07	_
ATOM	7968 OD2 ASP E 351	46.340 64.968 33.562 1.00 51.79	0
ATOM	7969 N ARGE 352	49.084 63.941 36.102 1.00 44.28	N
		50.397 64.373 35.671 1.00 44.89	
		51.454 63.293 35.758 1.00 45.67	
ATOM	7972 O ARGE 352	52.277 63.094 34.847 1.00 46.39	0
		50.791 65.599 36.479 1.00 45.31	
<b>ATOM</b>	7974 CG ARG E 352	50.074 66.823 35.923 1.00 47.04	С
ATOM	7975 CD ARG E 352	51.018 68.022 36.145 1.00 48.79	С
<b>ATOM</b>	7976 NE ARG E 352	50.749 68.361 37.541 1.00 51.41	N
ATOM	7977 CZ ARG E 352	51.710 68.620 38.432 1.00 52.42	C
<b>ATOM</b>	7978 NH1 ARG E 352	52.973 68.607 38.039 1.00 51.54	N
<b>ATOM</b>	7979 NH2 ARG E 352	51.239 68.883 39.656 1.00 53.39	N
		51.452 62.533 36.853 1.00 44.89	
		52.427 61.455 36.998 1.00 42.61	
<b>ATOM</b>	7982 C GLUE 353	52.225 60.407 35.922 1.00 41.58	С
ATOM	7983 O GLU E 353	53.165 59.738 35.520 1.00 41.66	0
ATOM	7984 CB GLU E 353	52.212 60.810 38.359 1.00 42.28	С
ATOM	7985 CG GLUE 353	52.159 61.796 39.504 1.00 42.55	С
ATOM	7986 CD GLUE 353	52.357 61.064 40.813 1.00 44.11	C
ATOM	7987 OE1 GLU E 353	53.418 60.438 40.997 1.00 44.30	0
		51.435 61.111 41.652 1.00 45.63	
		50.992 60.243 35.461 1.00 41.20	N
		50.638 59.265 34.459 1.00 41.40	
ATOM	7991 C LEUE 354	51.483 59.446 33.222 1.00 41.40	C
ATOM	7992 O LEUE 354	51.988 58.492 32.637 1.00 41.35 49.132 59.282 34.178 1.00 40.94	0
ATOM	7993 CB LEUE 354	49.132 59.282 34.178 1.00 40.94	C C
		48.423 58.370 35.199 1.00 40.08	
ATOM	7995 CD1 LEU E 354	46.976 58.751 35.290 1.00 39.80 48.644 56.929 34.750 1.00 40.20	C
		51.649 60.702 32.847 1.00 41.94	N
	7997 N VALE 355	52.492 60.999 31.680 1.00 42.07	C
	7999 CA VALE 355	53.888 60.446 31.901 1.00 43.39	c ·
	8000 O VALE 355	54.390 59.614 31.137 1.00 45.00	Ö
	8001 CB VALE 355	52.519 62.515 31.489 1.00 39.86	C
		53.353 62.849 30.312 1.00 40.48	C
		51.096 62.910 31.194 1.00 41.98	C
	8004 N HIS E 356		N
		55.870 60.352 33.297 1.00 44.05	C
	8006 C HIS E 356	55.863 58.844 33.379 1.00 43.90	C
	8007 O HISE 356	56,805 58,186 32,912 1.00 43,40	0
		56.329 61.010 34.606 1.00 48.13	C
		56.461 62.483 34.331 1.00 51.56	С

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		287/3/1	N
ATOM	8010 ND1 HIS E 356	57.666 63.111 34.140 1.00 53.20	N C
ATOM	8011 CD2 HIS E 356	55.505 63.431 34.182 1.00 53.15 57.444 64.386 33.886 1.00 54.09 56.142 64.614 33.906 1.00 54.08	C
ATOM	8012 CEI HIS E 356	5/,444 64,386 33.886 1.00 54.09	N
ATOM	8013 NE2 HIS E 356	54.803 58.280 33.973 1.00 43.77	N
ATOM	8014 N MET E 357	54.803 58.280 33.973 1.00 43.77	C
ATOM	8015 CA MET E 35/	54.698 56.845 34.125 1.00 42.63	c
ATOM	8016 C MET E 357	54.900 56.088 32.823 1.00 42.16	0
ATOM	8017 O MET E 357	55.651 55.134 32.758 1.00 42.72	C
ATOM	8018 CB MET E 357	53.379 56.351 34.719 1.00 42.21	
ATOM	8019 CG MET E 357	53.567 54.845 35.039 1.00 41.81	
ATOM	8020 SD MET E 357	52.012 54.208 35.644 1.00 41.75	S C
ATOM	8021 CE MET E 357	51.933 55.033 37.233 1.00 43.97	
ATOM	8022 N ILEE 358	54.191 56.505 31.800 1.00 42.02	N
ATOM	8023 CA ILE E 358	54.262 55.912 30.473 1.00 41.51	C
ATOM	8024 C ILE E 358	55.700 55.930 29.986 1.00 42.64	С
ATOM	8025 O ILEE 358	56.154 54.908 29.485 1.00 42.86	0.
ATOM	8026 CB ILE E 358	53.376 56.704 29.491 1.00 39.37	C
ATOM	8027 CG1 ILE E 358	51.923 56.606 29.934 1.00 38.89 53.525 56.159 28.096 1.00 38.83 50.944 57.324 29.059 1.00 38.55 56.391 57.053 30.131 1.00 44.20	C
ATOM	8028 CG2 ILE E 358	53.525 56.159 28.096 1.00 38.83	C
ATOM	8029 CD1 ILE E 358	50.944 57.324 29.059 1.00 38.55	C N
ATOM	8030 N ASN E 359	56.391 57.053 30.131 1.00 44,20	N
ATOM	8031 CA ASN E 359	57.787 57.136 29.737 1.00 46.66	C
ATOM	8032 C ASN E 359	58.658 56.162 30.509 1.00 45.71 59.451 55.383 29.997 1.00 46.33	C
ATOM	8033 O ASN E 359	59.451 55.383 29.997 1.00 46.33	0
ATOM	8034 CB ASN E 359	58.293 58.549 30.031 1.00 51.90	C C
ATOM	8035 CG ASN E 359	57.759 59.447 28.926 1.00 55.87	
ATOM	8036 OD1 ASN E 359	58.138 59.117 27.792 1.00 59.61	N
ATOM	8037 ND2 ASN E 359	58.138 59.117 27.792 1.00 59.61 56.958 60.463 29.184 1.00 56.96	N,
ATOM	8038 N TRP E 360	58.512 56.147 31.823 1.00 44.20	14
ATOM	8039 CA TRP E 360	59.254 55.214 32.656 1.00 42.84	C
		59.039 53.781 32.220 1.00 42.98	
	8041 O TRP E 360		0
	8042 CB TRP E 360		C C
	8043 CG TRP E 360	59.076 54.246 34.936 1.00 42.93	
	8044 CD1 TRP E 360	60.296 54.048 35.506 1.00 42.78	C
	8045 CD2 TRP E 360	58.243 53.141 35.326 1.00 42.85	C
	8046 NE1 TRP E 360		N
	8047 CE2 TRP E 360		С
ATOM	8048 CE3 TRP E 360	56.918 52.787 35.049 1.00 42.24	C
		58.547 51.142 36.704 1.00 41.92	C
	8050 CZ3 TRP E 360	56.453 51.623 35.608 1.00 43.00	C
	8051 CH2 TRP E 360	57.261 50.814 36.418 1.00 42.73	C
	8052 N ALA E 361	57.799 53.369 31.978 1.00 44.16	N
	8053 CA ALA E 361	57.451 52.023 31.565 1.00 44.49	C
ATOM	8054 C ALA E 361	58.326 51.629 30.391 1.00 45.81	С

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ΔΤΟΜ	8055 O ALA E 361	•	0
		55.998 51.877 31.146 1.00 43.81	C
ATOM ATOM	8057 N LYS E 362	58.497 52.519 29.414 1.00 48.10	N
ATOM	8058 CA LYS E 362	59.294 52.228 28.240 1.00 51.06	С
	8059 C LYS E 362		С
	8060 O LYSE 362	61.285 51.122 27.659 1.00 52.51	0
		59.220 53.381 27.248 1.00 52.88	С
<b>ATOM</b>	8062 CG LYS E 362	57.815 53.499 26.670 1.00 56.32	С
<b>ATOM</b>	8063 CD LYS E 362	57.545 52.350 25.706 1.00 59.44	С
ATOM	8064 CE LYS E 362	56,994 52,840 24,368 1.00 62.09	C .
ATOM	8065 NZ LYS E 362	56.986 51.784 23.287 1.00 63.02	N
<b>ATOM</b>	8066 N ARG E 363	61.327 52.195 29.615 1.00 52.40	N
		62.665 51.847 30.003 1.00 53.85	С
	8068 C ARG E 363		C
	8069 O ARG E 363		0
	8070 CB ARG E 363		C
ATOM	8071 CG ARG E 363	62.449 54.263 30.564 1.00 62.85	C
ATOM	8072 CD ARG E 363	62.981 54.929 29.283 1.00 68.62	C
ATOM	8073 NE ARGE 363	64.337 55.368 29.657 1.00 74.45	
		64.512 56.355 30.546 1.00 77.99	C
		63,433 56,948 31,074 1,00 79,59	N N
		65.754 56.721 30.882 1.00 79.71 61.687 49.981 31.340 1.00 51.00	N
	8077 N VALE 364	61.879 48.840 32.271 1.00 48.62	C.
		62.332 47.706 31.392 1.00 47.70	c
		61.613 47.311 30.477 1.00 48.86	Ö
ATOM	8081 CB VALE 364	60.540 48.512 32.969 1.00 47.56	C
		60.553 47.172 33.659 1.00 45.31	C
		60.173 49.655 33.902 1.00 47.17	С
		63.501 47.189 31.585 1.00 47.26	N
		64.060 46.117 30.774 1.00 47.42	С
	8086 C PRO E 365	63.036 45.052 30.471 1.00 48.06	С
	8087 O PRO E 365	62.452 44.562 31.429 1.00 48.89	Ο
<b>ATOM</b>	8088 CB PRO E 365	65.247 45.558 31.568 1.00 47.14	С
	8089 CG PRO E 365	65.708 46.873 32.187 1.00 48.39	C
	8090 CD PRO E 365	64.443 47.641 32.608 1.00 48.24	С
	8091 N GLY E 366	62.811 44.736 29.191 1.00 48.05	N
	8092 CA GLY E 366	61.888 43.705 28.785 1.00 46.86	<b>C</b> .
	8093 C GLY E 366	60.530 44.191 28.352 1.00 47.67	C
	8094 O GLY E 366	59.827 43.546 27.556 1.00 48.69	0
	8095 N PHE E 367	60.102 45.339 28.867 1.00 47.11	N
	8096 CA PHE E 367	58.791 45.899 28.567 1.00 46.48	C
	8097 C PHE E 367	58.503 46.101 27.083 1.00 46.37 57.541 45.710 26.434 1.00 45.46	C
	8098 O PHE E 367	57.541 45.719 26.424 1.00 45.46	O C
ATOM	8099 CB PHE E 367	58.659 47.258 29.288 1.00 45.29	C

wo	98/568	12	,	PCT
			) 89/37I	
ATOM	8100	CG PHE E 367		С
ATOM		CD1 PHE E 367		С
		CD2 PHE E 367	56.941 48.862 28.393 1.00 46.15	С
		CEI PHE E 367	54.949 47.675 29.873 1.00 45.31	С
		CE2 PHE E 367	55.650 49.347 28.314 1.00 46.17	С
		CZ PHE E 367	54.648 48.755 29.064 1.00 45.75	С
		N VALE 368	59.433 46.793 26.454 1.00 46.85	N
		CA VALE 368	59.418 47.174 25.063 1.00 47.56	C
ATOM	8108	C VALE 368	59.401 45.970 24.147 1.00 49.50	С
<b>ATOM</b>	8109	O VAL E 368	58.958 46.117 22.986 1.00 51.13	0
<b>ATOM</b>	8110	CB VALE 368	60.621 48.100 24.855 1.00 46.24	С
<b>ATOM</b>	8111	CG1 VAL E 368	61.431 47.684 23.666 1.00 46.91	C
<b>ATOM</b>	8112	<b>CG2 VAL E 368</b>	60.060 49.501 24.798 1.00 46.71	С
		N ASP E 369	59.830 44.797 24.609 1.00 49.22	N
			59.748 43.611 23.791 1.00 49.90	С
		C ASP E 369		C
		O ASP E 369		0
			60.551 42.440 24.356 1.00 53.57	C
		CG ASP E 369	62.001 42.767 24.627 1.00 57.64	C
		OD1 ASP E 369	62.632 43.529 23.837 1.00 59.82	0
		OD2 ASP E 369	62.486 42.232 25.664 1.00 58.81	0
		N LEUE 370	57.282 43.617 24.298 1.00 46.26	N
		CA LEUE 370	•	C
		C LEUE 370		C O
		O LEUE 370		C
			55.220 43.372 25.525 1.00 44.62 55.824 42.653 26.729 1.00 43.72	C
			55.091 42.990 28.001 1.00 43.76	C
			55.711 41.158 26.484 1.00 44.23	Č
			54.118 43.310 22.554 1.00 42.71	N
			53.471 44.056 21.474 1.00 42.93	C
		C THRE 371	52.959 45.372 21.994 1.00 43.15	C
		O THR E 371	52.609 45.480 23.152 1.00 42.85	O
		CB THR E 371	52.262 43.256 20.975 1.00 43.47	С
		OG1 THR E 371	51.545 42.926 22.173 1.00 44.71	O
		CG2 THR E 371	52,704 41.986 20.277 1.00 43.38	С
		N LEU E 372	52.865 46.372 21.118 1.00 45.22	N
<b>ATOM</b>	8137	CA LEUE 372	52.359 47.690 21.532 1.00 44.77	С
<b>ATOM</b>	8138	C LEU E 372	51.069 47.563 22.338 1.00 45.09	C
<b>ATOM</b>	8139	O LEU E 372	50.957 48.200 23.398 1.00 44.44	Ο
ATOM	8140	CB LEUE 372	52.234 48.576 20.295 1.00 42.49	С
ATOM	8141	CG LEU E 372	53.548 48.903 19.617 1.00 41.22	С
ATOM	8142	CD1 LEU E 372	53.264 49.684 18.350 1.00 43.25	C
			54.427 49.746 20.512 1.00 41.76	С
ATOM	8144	N HIS E 373	50.106 46.745 21.912 1.00 45.43	N

C 48.884 46.647 22.706 1.00 47.32 ATOM 8145 CA HIS E 373 ATOM 8146 C HISE 373 49.173 46.044 24.067 1.00 47.30 48.655 46.557 25.084 1.00 46.34 ATOM 8147 O HISE 373 0 ATOM 8148 CB HIS E 373 47.801 45.952 21.902 1.00 49.96 C C 47.251 46.889 20.863 1.00 53.52 ATOM 8149 CG HIS E 373 47.573 46.867 19.519 1.00 54.14 N ATOM 8150 ND1 HIS E 373 C 46.370 47.908 21.001 1.00 54.57 ATOM 8151 CD2 HIS E 373 C ATOM 8152 CE1 HIS E 373 46.907 47.824 18.904 1.00 54.87 ATOM 8153 NE2 HIS E 373 46.166 48.494 19.778 1.00 55.54 N ATOM 8154 N ASP E 374 50.019 45.003 24.138 1.00 46.26 N ATOM 8155 CA ASP E 374 50.307 44.485 25.479 1.00 46.26 C ATOM 8156 C ASP E 374 50.909 45.514 26.420 1.00 45.67 C ATOM 8157 O ASP E 374 50.611 45.500 27.626 1.00 45.81 0 ATOM 8158 CB ASP E 374 51.139 43.207 25.389 1.00 47.09 C ATOM 8159 CG ASP E 374 50.122 42.191 24.898 1.00 49.52 C 0 ATOM 8160 OD1 ASP E 374 48.918 42.529 24.963 1.00 49.64 ATOM 8161 OD2 ASP E 374 50.503 41.088 24.455 1.00 53.31 0 ATOM 8162 N GLN E 375 51.740 46.411 25.899 1.00 44.54 N ATOM 8163 CA GLN E 375 52.289 47.443 26.773 1.00 44.93 C 51.124 48.252 27.326 1.00 45.36 C ATOM 8164 C GLN E 375 ATOM 8165 O GLN E 375 50.974 48.358 28.552 1.00 46.12 0 ATOM 8166 CB GLN E 375 53.267 48.293 25.992 1.00 44.78 C C ATOM 8167 CG GLN E 375 54.412 47.413 25.523 1.00 46.26 C ATOM 8168 CD GLN E 375 55.356 48.147 24.606 1.00 46.81 55.540 49.358 24.681 1.00 47.74 0 ATOM 8169 OE1 GLN E 375 ATOM 8170 NE2 GLN E 375 55.949 47.353 23.742 1.00 47.03 N ATOM 8171 N VALE 376 50.261 48.767 26.442 1.00 44.88 N ATOM 8172 CA VALE 376 49.094 49.513 26.906 1.00 43.54 C ATOM 8173 C VALE 376 48.332 48.676 27.929 1.00 43.22 C ATOM 8174 O VALE 376 0 47.948 49.192 28.975 1.00 43.63 ATOM 8175 CB VALE 376 48.174 49.957 25.768 1.00 43.24 C ATOM 8176 CG1 VAL E 376 47.227 51.017 26.293 1.00 44.01 ATOM 8177 CG2 VAL E 376 48.960 50.549 24.615 1.00 41.99 C ATOM 8178 N HIS E 377 48.120 47.391 27.711 1.00 43.66 N ATOM 8179 CA HIS E 377 47.416 46.562 28.698 1.00 44.10 C C ATOM 8180 C HIS E 377 48.161 46.583 30.004 1.00 43.06 ATOM 8181 O HIS E 377 47.596 47.052 30.994 1.00 43.74 0 ATOM 8182 CB HIS E 377 47.186 45.144 28.150 1.00 45.65 C ATOM 8183 CG AHIS E 377 46.526 44.179 29.078 0.50 44.17 C ATOM 8184 CG BHIS E 377 46.100 45.198 27.098 0.50 48.43 ATOM 8185 ND1AHIS E 377 45.200 44.280 29.448 0.50 43.92 N ATOM 8186 ND1BHIS E 377 46.290 44.797 25.788 0.50 48.69 N ATOM 8187 CD2AHIS E 377 47.005 43.091 29.723 0.50 44.07 C C ATOM 8188 CD2BHIS E 377 44.810 45.630 27.175 0.50 49.00 C ATOM 8189 CE1AHIS E 377 44.898 43.302 30.282 0.50 43.39

ATOM 8234 CG TRP E 383

wo	98/56812	292/371	PCT/GB98/01708
		292/371	
ATOM	8235 CD1 TRP E 383	45.367 52.465 35.652 1.00 37.08	C
ATOM	8236 CD2 TRP E 383	45.753 54.280 36.919 1.00 38.22	C
ATOM	8237 NEI TRP E 383	44.154 52.898 36.133 1.00 37.35	IN C
ATOM	8238 CE2 TRP E 383	44.361 54.007 36.924 1.00 38.41	C
		46.244 55.367 37.659 1.00 37.25	
ATOM	8240 CZ2 TRP E 383	43.472 54.816 37.635 1.00 37.58	C
ATOM	8241 CZ3 TRP E 383	45.347 56.146 38.354 1.00 36.24	С
ATOM	8242 CH2 TRP E 383	43.979 55.875 38.321 1.00 36.44	C
ATOM	8243 N LEUE 384	47.314 52.548 38.843 1.00 37.45	N ·
ATOM	8244 CA LEU E 384	47.090 52.912 40.242 1.00 35.59	C
ATOM	8245 C LEU E 384	47.983 52.128 41.184 1.00 35.15	C
ATOM	8246 O LEUE 384	48.381 52.659 42.213 1.00 33.91	0
ATOM	8247 CB LEUE 384	45.600 52.817 40.542 1.00 34.80	C
ATOM	8248 CG LEU E 384	45.114 53.321 41.892 1.00 35.29	C
ATOM	8249 CD1 LEU E 384	45.618 54.739 42.208 1.00 35.78	C
ATOM	8250 CD2 LEU E 384	43.596 53.340 41.977 1.00 33.47	C
		48.354 50.871 40.891 1.00 36.22	
ATOM	8252 CA GLU E 385	49.202 50.124 41.837 1.00 35.99	С
ATOM	8253 C GLUE 385	50.530 50.872 41.839 1.00 35.17	С
ATOM	8254 O GLUE 385	51.029 51.208 42.902 1.00 34.47	0
		49.349 48.648 41.567 1.00 36.38	
<b>ATOM</b>	8256 CG GLUE 385	48.330 47.663 42.046 1.00 37.25	C
<b>ATOM</b>	8257 CD GLUE 385	48.535 46.270 41.481 1.00 39.83 48.115 46.085 40.310 1.00 39.19	С
ATOM	8258 OE1 GLU E 385	48.115 46.085 40.310 1.00 39.19	О
		49.090 45.352 42.167 1.00 42.19	0
ATOM	8260 N ILE E 386	51.042 51.136 40.638 1.00 35.91	N
<b>ATOM</b>	8261 CA ILE E 386	52.295 51.859 40.493 1.00 36.84 52.198 53.189 41.248 1.00 37.39	С
ATOM	8262 C ILE E 386	52.198 53.189 41.248 1.00 37.39	C
		53.101 53.418 42.031 1.00 37.87	
		52.733 52.263 39.081 1.00 37.29	
		52.655 51.193 38.000 1.00 39.11	
	8266 CG2 ILE E 386	54.153 52.766 39.108 1.00 36.98	C
	8267 CD1 ILE E 386	53.450 49.952 38.250 1.00 40.93	C
	8268 N LEUE 387	51.181 54.024 41.039 1.00 37.44	N
	8269 CA LEUE 387	51.079 55.276 41.749 1.00 36.84	<b>C</b>
	8270 C LEUE 387	51.104 55.057 43.250 1.00 37.11	C
	8271 O LEUE 387	51.809 55.773 43.946 1.00 37.83	0
ATOM	8272 CB LEUE 387	49.787 56.045 41.473 1.00 37.36	C
ATOM	8273 CG LEU E 387	49.672 56.828 40.166 1.00 38.07	C
<b>ATOM</b>	8274 CD1 LEU E 387	48.281 57.449 40.044 1.00 37.57	С
	8275 CD2 LEU E 387	50.758 57.878 40.028 1.00 37.61	С
ATOM	8276 N MET E 388	50.345 54.083 43.735 1.00 37.87	N
ATOM	8277 CA MET E 388	50.270 53.824 45.165 1.00 37.01	С
<b>ATOM</b>	8278 C MET E 388	51.599 53.354 45.697 1.00 37.19	С
ATOM	8279 O MET E 388	51.935 53.886 46.766 1.00 38.13	0

C

ATOM 8414 CE2 PHE E 404 47.838 60.888 47.541 1.00 44.40

47.889 61.924 49.695 1.00 46.11

ATOM 8413 CE1 PHE E 404

			2 -01	
			47.400 60.966 48.842 1.00 45.60	С
ATOM	8416	N ALA E 405	53.213 64.996 47.448 1.00 49.95	N
ATOM	8417	CA ALA E 405	54.261 65.757 46.787 1.00 52.59	C
		C ALA E 405	55.197 66.307 47.835 1.00 53.64	С
			54.871 66.317 49.018 1.00 55.50	0
<b>ATOM</b>	8420	CB ALA E 405	53.650 66.938 46.034 1.00 53.32	С
<b>ATOM</b>	8421	N PRO E 406	56.315 66.857 47.408 1.00 54.23	N
<b>ATOM</b>	8422	CA PRO E 406	57.308 67.482 48.284 1.00 54.34	С
<b>ATOM</b>	8423	C PRO E 406	56.574 68.626 48.967 1.00 54.49	С
ATOM	8424	O PRO E 406	56.811 68.813 50.148 1.00 56.57	Ο
ATOM	8425	CB PRO E 406	58.508 67.936 47.470 1.00 53.22	С
ATOM	8426	CG PRO E 406 -	58.228 67.270 46.164 1.00 53.88	С
<b>ATOM</b>	8427	CD PRO E 406	56.744 66.938 46.023 1.00 54.30	С
<b>ATOM</b>	8428	N ASN E 407	55.682 69.300 48.272 1.00 53.76	N
<b>ATOM</b>	8429	CA ASN E 407	54.909 70.361 48.867 1.00 54.30	С
<b>ATOM</b>	8430	C ASN E 407	53.465 69.995 49.121 1.00 55.11	С
<b>ATOM</b>	8431	O ASN E 407	52.622 70.904 49.123 1.00 56.53	Ο
			55.011 71.560 47.924 1.00 55.00	С
<b>ATOM</b>	8433	CG ASN E 407	54.181 71.361 46.688 1.00 55.76	С
			54.138 70.284 46.113 1.00 57.06	0
			53.492 72.405 46.279 1.00 57.34	N
			53.107 68.731 49.307 1.00 55.09	
			51.700 68.394 49.595 1.00 54.77	
		C LEU E 408		C
			52.083 66.123 50.085 1.00 56.28	0
			50.797 68.071 48.453 1.00 53.54	С
<b>ATOM</b>	8441		49.357 67.658 48.721 1.00 52.83	С
			48.613 68.523 49.692 1.00 51.64	С
			48.579 67.655 47.396 1.00 53.46	C
			51.637 67.479 51.860 1.00 56.09	N
			51.790 66.390 52.829 1.00 55.60	C
			50.546 66.225 53.671 1.00 55.76	С
		O LEU E 409	50.441 66.799 54.737 1.00 56.37	0
		CB LEU E 409	53.027 66.737 53.616 1.00 55.29	С
		CG LEU E 409	53.557 65.981 54.811 1.00 54.70	C
		CD1 LEU E 409	53.370 64.493 54.726 1.00 54.26	C
		CD2 LEU E 409	55.061 66.263 54.928 1.00 55.29	С
		N LEUE 410	49.574 65.443 53.205 1.00 56.47	N
		CA LEUE 410	48.342 65.262 53.952 1.00 56.35	С
		C LEUE 410	48.637 64.342 55.114 1.00 58.87	C
		O LEUE 410	49.603 63.582 55.135 1.00 59.73	o
		CB LEUE 410	47.193 64.774 53.099 1.00 54.74	C
		CG LEU E 410	47.035 65.606 51.825 1.00 54.12	C
			45.915 65.082 50.962 1.00 54.60	C
ATOM	8459	CD2 LEU E 410	46.804 67.054 52.215 1.00 53.95	С

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ATOM	8505 CG LYS E 416	38.708 62.042 58.641 1.00 74.66	С
ATOM	8506 CD LYS E 416	37.872 61.379 59.724 1.00 77.68 38.165 61.959 61.103 1.00 80.25	С
<b>ATOM</b>	8507 CE LYS E 416	38.165 61.959 61.103 1.00 80.25	С
ATOM	8508 NZ LYS E 416	39.365 61.334 61.753 1.00 82.62	N
		38.193 64.535 54.744 1.00 67.34	
		37.629 65.560 53.895 1.00 67.24	C
	8511 C CYS E 417		C
		35.771 65.380 52.469 1.00 66.59	0
ATOM	8513 CB CYS E 417	38.722 66.539 53.457 1.00 69.38	C S
ATOM	8514 SG CYSE 417	39.355 67.479 54.900 1.00 74.04	
		37.350 63.853 52.141 1.00 63.31 36.658 63.184 51.054 1.00 60.57	
ATOM	9517 C VALE 418	35.994 61.907 51.541 1.00 60.34	c
ATOM	8518 O VALE 418	36.608 61.182 52.293 1.00 59.16	Ö
ATOM	8519 CR VALE 418	37.604 62.859 49.901 1.00 59.16	Č
		36.927 62.062 48.805 1.00 58.97	Č
		38.147 64.151 49.318 1.00 58.63	C
		34.773 61.664 51.136 1.00 62.30	N
		33.967 60.513 51.471 1.00 65.39	С
<b>ATOM</b>	8524 C GLUE 419	34.668 59.207 51.171 1.00 64.79	С
		35.275 58.988 50.122 1.00 65.46	0
ATOM	8526 CB GLU E 419	32.700 60.554 50.628 1.00 70.25	С
ATOM	8527 CG GLUE 419	31.397 60.207 51.316 1.00 76.71	C
		30.289 59.850 50.330 1.00 80.65	
ATOM	8529 OE1 GLU E 419	30.259 60.410 49.200 1.00 82.59	
		29.420 58.996 50.660 1.00 82.71	0
		34.663 58.263 52.095 1.00 63.96	N C
		35.329 57.000 51.876 1.00 63.44 36.825 56.991 51.685 1.00 62.43	
ATOM	8534 O GIVE 420	37.362 55.901 51.460 1.00 63.54	o
	8535 N MET E 421	37.589 58.040 51.788 1.00 61.69	N
	8536 CA MET E 421	39.015 58.104 51.653 1.00 61.14	C
	8537 C MET E 421		C
		41.021 57.282 52.649 1.00 60.75	0
	8539 CB MET E 421	39.400 59.586 51.439 1.00 62.19	С
ATOM	8540 CG MET E 421	39.464 59.848 49.952 1.00 63.76	С
	8541 SD MET E 421	41.214 59.747 49.509 1.00 64.70	S
	8542 CE MET E 421	41.583 61.487 49.813 1.00 65.67	C
	8543 N VALE 422	39.411 57.829 54.048 1.00 60.12	N
	8544 CA VAL E 422	40.143 57.500 55.249 1.00 59.26	С
	8545 C VALE 422	40.593 56.051 55.239 1.00 58.74	C
	8546 O VALE 422	41.732 55.886 55.666 1.00 58.75	0
	8547 CB VALE 422	39.340 57.632 56.564 1.00 59.81	C C
		40.170 58.363 57.610 1.00 60.12 38.025 58.347 56.309 1.00 60.75	C
AIUM	6349 CGZ VAL E 422	36.023 36.347 36.309 1.00 60.73	C

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ATOM	8550 N GLUE 423	39.739 55.125 54.804 1.00 57.81	N
ATOM	8551 CA GLUE 423	40.127 53.727 54.792 1.00 58.23	С
	8552 C GLU E 423		С
ATOM	8553 O GLUE 423	42.217 52.767 54.120 1.00 54.90	0
ATOM	8554 CB GLUE 423	39.014 52.779 54.396 1.00 63.04	C
ATOM	8555 CG GLUE 423	37.777 52.932 55.260 1.00 69.79	C
ATOM	8556 CD GLUE 423	36.871 54.029 54.697 1.00 74.22	C
ATOM	8557 OE1 GLU E 423	37.159 55.247 54.849 1.00 74.78	
		35.839 53.636 54.066 1.00 77.24	O N
ATOM	8559 N ILEE 424	41.175 54.147 52.664 1.00 51.41	C
ATOM	8560 CA ILEE 424	42.266 54.040 51.697 1.00 47.98	C
ATOM	8301 C ILEE 424	43.493 54.655 52.339 1.00 48.22 44.569 54.017 52.381 1.00 49.81	Ö
ATOM	8563 CR II F F 424	41.809 54.691 50.412 1.00 46.43	
ATOM	8564 CG1 II F F 424	40.626 53.844 49.916 1.00 45.58	C
ATOM	8565 CG2 ILEE 424	42.919 54.746 49.387 1.00 46.53	Ċ
		39.973 54.492 48.721 1.00 45.49	
ATOM	8567 N PHE E 425	43.404 55.835 52.944 1.00 46.64	N
ATOM	8568 CA PHE E 425	44.559 56.416 53.614 1.00 46.97	С
	8569 C PHE E 425		С
<b>ATOM</b>	8570 O PHE E 425	46.309 55.306 54.875 1.00 48.59	Ο
<b>ATOM</b>	8571 CB PHE E 425	44.198 57.739 54.285 1.00 46.71	C
<b>ATOM</b>	8572 CG PHE E 425	44.315 58.934 53.392 1.00 46.51	C
ATOM	8573 CD1 PHE E 425	44.121 58.804 52.022 1.00 47.41	C
ATOM	8574 CD2 PHE E 425	44.606 60.166 53.908 1.00 45.89	C
ATOM	8575 CE1 PHE E 425	44.226 59.870 51.169 1.00 47.79	C
ATOM	8576 CE2 PHE E 425	44.713 61.243 53.061 1.00 47.82	C C
ATOM	8577 CZ PHEE 425	44.533 61.114 51.689 1.00 48.33	N
		44.209 54.801 55.378 1.00 49.18 44.641 53.882 56.435 1.00 50.32	C
	8580 C ASP E 426		
	8581 O ASP E 426	46.560 52.514 56.382 1.00 50.94	Ö
	8582 CB ASP E 426	43,444 53,475 57,263 1.00 52.85	C
	8583 CG ASP E 426		С
	8584 OD1 ASP E 426	44.105 55.313 58.581 1.00 56.03	0
	8585 OD2 ASP E 426	42.050 54.547 58.918 1.00 55.96	0
	8586 N MET E 427	45.012 52.091 54.829 1.00 48.06	N
<b>ATOM</b>	8587 CA MET E 427	45.745 51.025 54.169 1.00 45.93	С
	8588 C MET E 427	47.068 51.572 53.631 1.00 44.99	C
	8589 O MET E 427	48.142 50.951 53.764 1.00 44.81	0
	8590 CB MET E 427	44.866 50.475 53.055 1.00 46.28	C
	8591 CG MET E 427	43.702 49.673 53.618 1.00 47.12	C
	8592 SD MET E 427		S C
	8593 CE MET E 427		N N
ATOM	8594 N LEUE 428	47.014 52.774 53.049 1.00 42.52	14

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ATOM	8595 CA LEUE 428	48.268 53.339 52.557 1.00 41.97	С
ATOM	8596 C LEUE 428	49.234 53.533 53.710 1.00 42.31 50.398 53.126 53.571 1.00 43.27	С
ATOM	8597 O LEUE 428	50.398 53.126 53.571 1.00 43.27	0
ATOM	8598 CB LEU E 428	48.026 54.630 51.795 1.00 41.62	C
ATOM	8599 CG LEU E 428	47.304 54.478 50.452 1.00 40.23	С
ATOM	8600 CD1 LEU E 428	46.808 55.825 49.983 1.00 39.61 48.271 53.875 49.453 1.00 40.11	C
ATOM	8601 CD2 LEU E 428	48.271 53.875 49.453 1.00 40.11	С
		48.784 54.097 54.832 1.00 42.32	
ATOM	8603 CA LEUE 429	49.695 54.316 55.966 1.00 42.13	С
ATOM	8604 C LEUE 429	50.303 53.027 56.474 1.00 41.73	C
ATOM	8605 O LEUE 429	51.522 52.889 56.618 1.00 42.13	0
		48.997 55.122 57.050 1.00 42.21	
ATOM	8607 CG LEUE 429	48.743 56.587 56.666 1.00 42.47	C
ATOM	9600 CD2 LEUE 429	47.706 57.199 57.578 1.00 42.17 50.006 57.426 56.642 1.00 42.12	C
ATOM	8610 N AT A E 420	49.476 52.023 56.684 1.00 41.47	N
ATOM	9611 CA AI AE 430	49.927 50.709 57.111 1.00 42.24	C
ATOM	8612 C ALAE 430	51.002 50.130 56.196 1.00 43.35	c
ATOM	8613 O ALAE 430	51.941 49.496 56.695 1.00 43.89	Ö
ATOM	8614 CB ALAE 430	48.738 49.757 57.062 1.00 42.20	
ATOM	8615 N THR E 431	50.863 50.314 54.877 1.00 42.68	N
ATOM	8616 CA THR E 431	51.886 49.788 53.990 1.00 42.40	С
ATOM	8617 C THR E 431	51.886 49.788 53.990 1.00 42.40 53.149 50.600 54.194 1.00 43.01	С
<b>ATOM</b>	8618 O THR E 431	54.267 50.100 54.270 1.00 42.66	0
<b>ATOM</b>	8619 CB THR E 431	51.500 49.991 52.523 1.00 42.40	С
ATOM	8620 OG1 THR E 431	50.165 49.495 52.408 1.00 43.64 52.445 49.277 51.594 1.00 42.04	0
ATOM	8621 CG2 THR E 431	52.445 49.277 51.594 1.00 42.04	С
ATOM	8622 N SER E 432	52.895 51.914 54.285 1.00 44.22	N
		54.030 52.832 54.444 1.00 45.72	
ATOM	8624 C SER E 432	54.857 52.445 55.656 1.00 45.62	
ATOM	8625 O SER E 432	56.078 52.366 55.656 1.00 44.84	0
		53,569 54.272 54.448 1.00 45.63	C O
		54.753 55.052 54.544 1.00 46.77 54.141 52.164 56.715 1.00 46.95	N
	8628 N SER E 433 8629 CA SER E 433	54.705 51.722 57.965 1.00 40.93	C
	8630 C SER E 433	55.450 50.400 57.864 1.00 50.55	C
	8631 O SER E 433	56.573 50.223 58.340 1.00 50.04	Ö
	8632 CB SER E 433	53.466 51.523 58.844 1.00 52.38	C
	8633 OG SER E 433	53.946 51.508 60.181 1.00 56.50	0
	8634 N ARGE 434	54.867 49.401 57.191 1.00 51.62	N
		55.543 48.117 57.014 1.00 52.03	С
	8636 C ARGE 434		С
	8637 O ARGE 434	57.810 47.709 56.557 1.00 51.44	0
	8638 CB ARG E 434		С
ATOM	8639 CG ARG E 434	55.424 45.815 55.995 1.00 56.12	С

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ATOM	8640 CD ARG E 434	54.742 44.525 56.408 1.00 59.27	С
ATOM	8641 NE ARG E 434	55 682 43 366 56 334 1 00 60.61	N
ATOM	8642 CZ ARG E 434	55.682 43.366 56.334 1.00 60.61 56.551 43.176 57.327 1.00 60.77	C
ATOM	8643 NH1 ARG E 434	56.504 44.063 58.319 1.00 61.70	N
		57.407 42.174 57.336 1.00 61.04	
ATOM	8645 N PHE E 435	56.857 49.236 55.241 1.00 53.65	N
ATOM	8646 CA PHE E 435	58.075 49.492 54.496 1.00 55.21	C
		59.110 50.101 55.429 1.00 57.28	С
		60.298 49.827 55.313 1.00 56.92	
ATOM	8649 CB PHE E 435	57.856 50.389 53.292 1.00 55.58	C
ATOM	8650 CG PHE E 435	57.346 49.723 52.044 1.00 55.83	С
ATOM	8651 CD1 PHE E 435	57.272 48.349 51.909 1.00 55.27	<b>C</b> .
ATOM	8652 CD2 PHE E 435	56.921 50.492 50.970 1.00 55.48	С
ATOM	8653 CE1 PHE E 435	56.791 47.753 50.771 1.00 54.62	С
ATOM	8654 CE2 PHE E 435	56.435 49.929 49.819 1.00 54.80	С
ATOM	8655 CZ PHE E 435	56.374 48.548 49.732 1.00 55.27	С
		58.667 50.933 56.369 1.00 59.99	
<b>ATOM</b>	8657 CA ARG E 436	59.564 51.547 57.333 1.00 62.20	С
<b>ATOM</b>	8658 C ARG E 436	60.182 50.457 58.189 1.00 62.86	С
		61.371 50.353 58.390 1.00 62.51	
		58.806 52.531 58.210 1.00 63.59	
<b>ATOM</b>	8661 CG ARG E 436	59.645 53.678 58.742 1.00 66.33	С
ATOM	8662 CD ARG E 436	58.855 54.573 59.699 1.00 68.41 57.704 55.162 59.009 1.00 70.77	С
<b>ATOM</b>	8663 NE ARG E 436	57.704 55.162 59.009 1.00 70.77	N
		56.438 54.917 59.357 1.00 71.97	
ATOM	8665 NH1 ARG E 436	56.195 54.113 60.387 1.00 72.22	N.
ATOM	8666 NH2 ARG E 436	55,429 55,469 58,682 1.00 72,49	N
ATOM	8667 N MET E 437	59.352 49.583 58.719 1.00 65.85	N
ATOM	8668 CA MET E 437	59.780 48.495 59.572 1.00 68.28	C
ATOM	8669 C MET E 437	60.781 47.598 58.902 1.00 66.41	C
		61.737 47.225 59.562 1.00 67.60	
		58,597 47.637 60.008 1.00 73.91	
	8672 CG MET E 437		C
	8673 SD MET E 437		S
	8674 CE MET E 437	55.761 46.302 60.604 1.00 84.74	C
	8675 N MET E 438	60.639 47.235 57.653 1.00 64.77	N
	8676 CA MET E 438	61.542 46.352 56.940 1.00 62.86	C
	8677 C MET E 438	62.758 47.063 56.394 1.00 62.06	C
	8678 O MET E 438	63.655 46.472 55.819 1.00 61.19	0
	8679 CB MET E 438	60.834 45.849 55.687 1.00 63.11	С
	8680 CG MET E 438	59.521 45.168 56.012 1.00 63.13	C S
	8681 SD MET E 438	59.094 44.081 54.691 1.00 64.84	S C
	8682 CE MET E 438	60.614 43.488 53.985 1.00 64.56	N
	8683 N ASNE 439	62.714 48.366 56.549 1.00 62.91	C
AIUM	8084 CA ASN £ 439	63.787 49.228 56.103 1.00 64.19	C

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ATOM	8730 N PHE E 445	62.973 48.969 46.192 1.00 45.85	N
ATOM	8731 CA PHE E 445	61.777 49.707 45.775 1.00 44.80	C
<b>ATOM</b>	8732 C PHE E 445	61.576 49.615 44.275 1.00 45.78	С
<b>ATOM</b>	8733 O PHE E 445	60.573 49.140 43.752 1.00 46.63	Ο
ATOM	8734 CB PHE E 445	61.848 51.154 46.205 1.00 43.02	С
<b>ATOM</b>	8735 CG PHE E 445	60.831 52.044 45.569 1.00 43.23	С
ATOM	8736 CD1 PHE E 445	59.476 51.796 45.716 1.00 44.18	С
ATOM	8737 CD2 PHE E 445	61.198 53.137 44.817 1.00 43.23	С
ATOM	8738 CE1 PHE E 445	58.511 52.599 45.142 1.00 43.74	С
<b>ATOM</b>	8739 CE2 PHE E 445	60.260 53.959 44.224 1.00 43.01	C
ATOM	8740 CZ PHE E 445	58.924 53.684 44.396 1.00 43.58	С
ATOM	8741 N VAL E 446	62.579 50.068 43.545 1.00 46.16	N
ATOM		62.630 50.077 42.088 1.00 45.68	С
ATOM	8743 C VAL E 446	62.362 48.707 41.495 1.00 46.43	С
<b>ATOM</b>	8744 O VAL E 446	61.741 48.586 40.426 1.00 47.33	0
ATOM	8745 CB VAL E 446	63.991 50.727 41.796 1.00 45.32	С
<b>ATOM</b>	8746 CG1 VAL E 446	64.914 49.963 40.872 1.00 45.72	C
<b>ATOM</b>	8747 CG2 VAL E 446	63.724 52.122 41.284 1.00 45.43	C
<b>ATOM</b>	8748 N CYS E 447	62.769 47.617 42.126 1.00 45.86	N
<b>ATOM</b>	8749 CA CYS E 447	62.510 46.308 41.588 1.00 47.15	С
<b>ATOM</b>	8750 C CYS E 447	61.044 45.938 41.706 1.00 47.41	С
<b>ATOM</b>	8751 O CYS E 447	60.444 45.386 40.804 1.00 47.17	Ο
<b>ATOM</b>	8752 CB CYS E 447	63.340 45.289 42.408 1.00 48.11	С
<b>ATOM</b>	8753 SG CYS E 447	65.012 45.131 41.773 1.00 48.83	S
<b>ATOM</b>	8754 N LEU E 448	60.468 46.211 42.884 1.00 48.29	N
<b>ATOM</b>	8755 CA LEU E 448	59.075 45.863 43.186 1.00 46.52	С
<b>ATOM</b>	8756 C LEU E 448	58.158 46.558 42.207 1.00 44.79	С
<b>ATOM</b>	8757 O LEU E 448	57.273 45.984 41.603 1.00 45.09	Ο
<b>ATOM</b>	8758 CB LEU E 448	58.711 46.262 44.602 1.00 46.56	С
<b>ATOM</b>	8759 CG LEUE 448		С
<b>ATOM</b>	8760 CD1 LEU E 448	58.865 46.048 47.051 1.00 49.15	С
<b>ATOM</b>	8761 CD2 LEU E 448	58.698 43.984 45.668 1.00 47.57	С
<b>ATOM</b>			N
		57.700 48.661 41.087 1.00 42.55	С
	8764 C LYS E 449	57.667 48.014 39.725 1.00 41.51	С
	8765 O LYS E 449	56.576 47.973 39.148 1.00 41.11	0
	8766 CB LYS E 449	58.259 50.070 41.163 1.00 43.23	С
	8767 CG LYS E 449	57.213 51.131 40.878 1.00 44.11	С
	8768 CD LYS E 449	57.814 52.207 40.038 1.00 45.17	С
	8769 CE LYS E 449	58.566 53.240 40.879 1.00 46.14	С
	8770 NZ LYS E 449	58.905 54.311 39.862 1.00 47.75	N
	8771 N SER E 450	58.762 47.480 39.200 1.00 41.28	N
	8772 CA SER E 450	58.747 46.784 37.917 1.00 41.19	C
	8773 C SER E 450	58.009 45.447 37.965 1.00 39.26	C
ATOM	8774 O SER E 450	57.345 45.088 37.013 1.00 38.89	0

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ATOM	8775 CB SER E 450	60.151 46.414 37.429 1.00 41.77	С
		60.812 47.665 37.489 1.00 45.16	
		58.116 44.741 39.066 1.00 37.81	N
		57.411 43.491 39.217 1.00 38.28	С
ATOM	8779 C ILE E 451	55.942 43.845 39.068 1.00 38.66	С
<b>ATOM</b>	8780 O ILE E 451	55.260 43.153 38.304 1.00 39.09	0
ATOM	8781 CB ILE E 451	57.677 42.804 40.566 1.00 39.44	С
		59.159 42.383 40.551 1.00 40.75	
ATOM	8783 CG2 ILE E 451	56.735 41.649 40.826 1.00 36.95	С
ATOM	8784 CD1 ILE E 451	59.537 41.446 41.683 1.00 42.44 55.482 44.895 39.773 1.00 38.03	С
<b>ATOM</b>	8785 N ILE E 452	55.482 44.895 39.773 1.00 38.03	N
		54.077 45.292 39.670 1.00 36.73	
		53.667 45.590 38.228 1.00 37.55	
		52.630 45.154 37.740 1.00 37.79	
		53.778 46.525 40.539 1.00 35.25	
ATOM	8790 CG1 ILE E 452	54.042 46.194 41.990 1.00 34.33	C
ATOM	8791 CG2 ILE E 452	52.343 46.998 40.308 1.00 35.46 53.496 47.137 43.035 1.00 33.49	C
ATOM	8792 CD1 ILE E 452	53.496 47.137 43.035 1.00 33.49	C
		54.469 46.343 37.480 1.00 37.40	
ATOM	8794 CA LEU E 453	54.144 46.673 36.120 1.00 37.51	С
ATOM	8795 C LEUE 453	54.016 45.399 35.317 1.00 39.84 53.143 45.302 34.468 1.00 41.15	C
ATOM	8796 O LEUE 453	53.143 45.302 34.468 1.00 41.15	0
		55.216 47.577 35.480 1.00 36.14	
		55.078 47.731 33.950 1.00 34.66 53.789 48.461 33.614 1.00 33.30	
ATOM	8800 CD2 LEUE 453	56.293 48.419 33.373 1.00 33.44	C C
		54.913 44.438 35.483 1.00 42.17	
		54.884 43.238 34.678 1.00 43.70	
		53.940 42.135 35.110 1.00 44.73	
		53.478 41.386 34.231 1.00 45.81	
ATOM	8805 CB LEU E 454	56.313 42.619 34.636 1.00 43.59	C
		57.256 43.422 33.739 1.00 44.11	С
	8807 CD1 LEU E 454	58.696 43.048 34.044 1.00 44.82	С
	8808 CD2 LEU E 454	56.946 43.117 32.280 1.00 44.72	С
<b>ATOM</b>	8809 N ASN E 455	53.681 41.966 36.397 1.00 44.67	$\mathbf{N}$
<b>ATOM</b>	8810 CA ASN E 455	52.869 40.827 36.797 1.00 45.18	С
<b>ATOM</b>	8811 C ASN E 455	51.424 41.141 36.932 1.00 47.23	С
<b>ATOM</b>	8812 O ASN E 455	50.636 40.216 36.942 1.00 48.88	0
<b>ATOM</b>	8813 CB ASN E 455	53.419 40.284 38.114 1.00 45.05	C
	8814 CG ASN E 455	52.544 39.391 38.943 1.00 44.88	С
	8815 OD1 ASN E 455	51.977 39.852 39.945 1.00 44.69	0
	8816 ND2 ASN E 455	52.423 38.128 38.532 1.00 45.24	N
	8817 N SER E 456	51.007 42.368 37.060 1.00 51.07	N
	8818 CA SER E 456	49.584 42.600 37.276 1.00 54.67	C
ATOM	8819 C SER E 456	48.726 42.201 36.124 1.00 57.34	. <b>C</b>

	0000 O SED E 456	47 720 41 494 36 251 1 00 60 01	0
	8820 U SER E 456	47.729 41.484 36.251 1.00 60.01	c
ATOM	8821 CB SER E 456	49.364 44.032 37.754 1.00 55.11	ŏ
		49.674 44.134 39.133 1.00 54.61 49.004 42.608 34.919 1.00 60.38	N
	8823 N GLYE 457		Ċ
ATOM		48.129 42.260 33.798 1.00 64.14	c
ATOM	8825 C GLY E 457		o
ATOM	8826 O GLY E 457	47.944 40.834 31.957 1.00 65.56	N
		49.425 40.210 33.596 1.00 67.97	C
ATOM	8828 CA VAL E 458	49.868 39.019 32.903 1.00 71.23	C
ATOM	8829 C VAL E 458		
ATOM		48.846 37.316 31.620 1.00 76.05	0
ATOM	8831 CB VAL E 458	51.173 38.474 33.487 1.00 70.27	C
ATOM		51.000 37.726 34.770 1.00 68.98	C
ATOM	8833 CG2 VAL E 458	51.843 37.570 32.447 1.00 70.96	C
		47.851 37.716 33.554 1.00 79.48	N
	8835 CA TYR E 459		С
ATOM	8836 C TYR E 459		С
ATOM		44.547 36.689 32.687 1.00 87.09	0
ATOM		46.188 36.205 34.719 1.00 85.54	C
ATOM		47.370 35.726 35.539 1.00 88.44	C
<b>ATOM</b>		48.111 36.698 36.204 1.00 89.50	C
<b>ATOM</b>			C
<b>ATOM</b>	8842 CE1 TYR E 459	49.219 36.275 36.876 1.00 90.68	C
<b>ATOM</b>	8843 CE2 TYR E 459	48.948 34.066 36.372 1.00 90.42	C
<b>ATOM</b>	8844 CZ TYR E 459	49.673 35.017 37.045 1.00 91.07	C
<b>ATOM</b>	8845 OH TYR E 459		0
<b>ATOM</b>	8846 N THR E 460		N
<b>ATOM</b>	8847 CA THR E 460	44.735 38.894 31.022 1.00 91.17	C
<b>ATOM</b>	8848 C THR E 460		C
<b>ATOM</b>	8849 O THR E 460	44.875 40.522 29.247 1.00 93.81	0
<b>ATOM</b>	8850 CB THR E 460	44.058 40.024 31.818 1.00 91.35	C
<b>ATOM</b>	8851 OG1 THR E 460	44.688 40.271 33.075 1.00 92.02	. 0.
<b>ATOM</b>	8852 CG2 THR E 460	42.622 39.640 32.135 1.00 91.98	С
<b>ATOM</b>	8853 N PHE E 461	46.098 38.646 29.038 1.00 94.55	N
<b>ATOM</b>	8854 CA PHE E 461	46.656 39.112 27.775 1.00 95.80	С
<b>ATOM</b>	8855 C PHE E 461	45.738 39.274 26.580 1.00 97.31	C
<b>ATOM</b>	8856 O PHE E 461	45.871 40.307 25.864 1.00 98.52	0
<b>ATOM</b>	8857 CB PHE E 461	47.952 38.328 27.466 1.00 94.82	С
ATOM	8858 CG PHE E 461	49.092 39.224 27.891 1.00 94.07	С
	8859 CD1 PHE E 461	48.944 40.596 27.851 1.00 94.00	C
	8860 CD2 PHE E 461	50.285 38.714 28.324 1.00 94.41	С
	8861 CE1 PHE E 461	49.941 41.453 28.227 1.00 94.40	С
	8862 CE2 PHE E 461	51.310 39.562 28.702 1.00 94.59	С
	8863 CZ PHE E 461	51.145 40.931 28.653 1.00 94.60	С
	8864 N THR E 465		N

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ATOM	8865 CA THR E 465	47.001 33.276 21.784 1.00127.92	С
		48.437 32.771 21.760 1.00126.90	C
		49.171 32.986 22.734 1.00127.57	O
<b>ATOM</b>	8868 CB THR E 465	46.057 32.091 21.526 1.00128.62	C
ATOM	8869 OG1 THR E 465	46.652 30.878 22.015 1.00128.85	O
ATOM	8870 CG2 THR E 465	45.724 31.947 20.051 1.00129.15	С
		48.894 32.147 20.677 1.00124.80	N
		50.282 31.668 20.608 1.00122.43	
		51.285 32.802 20.827 1.00120.18	C
		52.355 32.585 21.413 1.00120.09	0
		50.529 30.930 19.293 1.00122.67	
ATOM	8879 N LYSE 467	50.948 34.024 20.388 1.00116.78	N
ATOM	8880 CA LYSE 407	51.786 35.193 20.620 1.00113.09	C C
		51.642 35.514 22.114 1.00109.31 52.603 35.953 22.740 1.00109.27	
		51.418 36.396 19.772 1.00114.44	
ATOM	8884 CG LYS F 467	52.515 37.429 19.562 1.00115.60	C
ATOM	8885 CD LYS E 467	51.923 38.725 19.019 1.00117.06	Č
		52.094 38.930 17.523 1.00117.84	
ATOM	8887 NZ LYS E 467	51.291 40.110 17.040 1.00117.85	N
ATOM	8888 N SER E 468	50.467 35.264 22.689 1.00104.19	N
		50.220 35.488 24.095 1.00100.08	С
<b>ATOM</b>	8890 C SER E 468	51.034 34.533 24.965 1.00 96.75	С
		51.551 34.894 26.016 1.00 96.60	0
ATOM	8892 CB SER E 468	48.758 35.266 24.491 1.00100.27	С
		47.938 36.279 23.954 1.00101.24	
		51.138 33.294 24.504 1.00 92.82	
ATOM	8895 CA LEU E 469	51.890, 32.278 25.235 1.00 89.41	С
ATOM	8896 C LEUE 469	53.354 32.681 25.198 1.00 87.00	C
		54.092 32.455 26.147 1.00 86.58 51.628 30.888 24.663 1.00 89.70	O C
		53.784 33.307 24.111 1.00 84.85	N
		55.169 33.762 23.995 1.00 83.18	C
	8904 C GLU E 470		c
	8905 O GLU E 470		0
	8906 CB GLUE 470	55.541 33.829 22.538 1.00 87.28	C
	8907 CG GLUE 470		С
<b>ATOM</b>	8908 CD GLUE 470		C
<b>ATOM</b>	8909 OE1 GLU E 470	55.328 34.582 19.878 1.00 98.20	0
	8910 OE2 GLU E 470	56.911 36.135 20.052 1.00 98.08	0
	8911 N GLUE 471		N
	8912 CA GLUE 471	54.280 37.123 25.586 1.00 71.37	С
	8913 C GLUE 471		C
	8914 O GLUE 471		0
ATOM	8915 CB GLUE 4/1	53.037 37.965 25.326 1.00 69.94	С

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ΔΤΟΜ	8061 ND1 HIS F 476	55.162 34.427 34.699 1.00 62.16	N
ATOM	8962 CD2 HIS E 476	54.585 33.264 32.927 1.00 62.05	C
ATOM	8963 CE1 HIS E 476	53.841 34.236 34.733 1.00 62.92	С
ATOM	8964 NE2 HIS E 476	53.456 33.533 33.678 1.00 62.30	N
ATOM	8965 N ARG E 477	59.914 35.209 32.362 1.00 57.98	N
<b>ATOM</b>	8966 CA ARG E 477	61.342 35.220 32.256 1.00 58.02	С
ATOM	8967 C ARG E 477	61.969 36.454 32.867 1.00 55.67	C
ATOM	8968 O ARGE 477	62.922 36.364 33.622 1.00 56.06	0
ATOM	8969 CB ARGE 477	61.713 35.226 30.771 1.00 62.72	C
ATOM	8970 CG ARGE 477	62.916 34.325 30.544 1.00 68.93	C C
ATOM	8971 CD ARGE 4//	62.323 32.907 30.431 1.00 74.07	
ATOM	8972 NE ARGE 477	61.522 32.895 29.202 1.00 79.55 62.084 32.880 27.978 1.00 82.67	C
ATOM	89/3 CZ ARGE 4//	63.417 32.868 27.852 1.00 83.92	N
ATOM	8974 NH1 ARGE 477	61.270 32.874 26.912 1.00 83.54	N
ATOM	8076 N VALE 478	61.457 37.628 32.539 1.00 53.33	N
ATOM	8977 CA VALE 478	61.979 38.885 33.065 1.00 51.57	C
		61.718 38.952 34.560 1.00 51.33	С
		62.521 39.436 35.371 1.00 50.99	0
ATOM	8980 CB VAL E 478	61.318 40.058 32.342 1.00 51.59	С
ATOM	8981 CG1 VAL E 478	61.843 41.394 32.837 1.00 51.45	С
		61.567 39.870 30.849 1.00 52.54	С
		60.546 38.412 34.941 1.00 49.88	N
		60.155 38.337 36.338 1.00 48.08	C
ATOM	8985 C LEUE 479	61.167 37.502 37.124 1.00 49.08	C O
		61.475 37.835 38.287 1.00 49.48 58.738 37.807 36.523 1.00 44.80	C
		57.638 38.850 36.416 1.00 43.44	Č
ATOM	8080 CD11F11F 479	56.280 38.165 36.412 1.00 43.41	C
ATOM	8990 CD2 LEUE 479	57.664 39.894 37.513 1.00 42.27	C
ATOM		61.718 36.448 36.508 1.00 49.49	N
		62.721 35.659 37.214 1.00 50.30	С
	8993 C ASP E 480		С
	8994 O ASP E 480		0
		63.032 34.332 36.570 1.00 51.42	C
	8996 CG ASP E 480	61.883 33.364 36.553 1.00 53.00	C
	8997 OD1 ASP E 480	61.007 33.431 37.432 1.00 54.16	0
	8998 OD2 ASP E 480	61.807 32.498 35.653 1.00 54.42	0 .
	8999 N LYS E 481	64.294 37.214 36.236 1.00 51.72	N C
	9000 CA LYS E 481	65.507 38.038 36.234 1.00 54.39	C
	9001 C LYS E 481	65.403 39.049 37.363 1.00 52.96 66.364 39.147 38.115 1.00 53.28	0
	9002 O LYS E 481 9003 CB LYS E 481	65,793 38,730 34,903 1.00 58.02	C
		67.175 39.344 34.731 1.00 62.09	Č
	9004 CG ETS E 481		C

69.605 38.540 34.546 1.00 69.03 C ATOM 9006 CE LYS E 481 69.759 39.365 35.799 1.00 71.71 N ATOM 9007 NZ LYS E 481 ATOM 9008 N ILE E 482 64.252 39.720 37.470 1.00 51.11 N ATOM 9009 CA ILE E 482 64.085 40,703 38.535 1.00 48.85 C 64.168 40.007 39.872 1.00 47.88 C ATOM 9010 C ILE E 482 ATOM 9011 O ILE E 482 64.789 40.547 40.798 1.00 47.61 O 62.850 41.564 38.372 1.00 48.90 ATOM 9012 CB ILE E 482 62.979 42.430 37.114 1.00 49.83 C ATOM 9013 CG1 ILE E 482 C 62.686 42.515 39.541 1.00 48.66 ATOM 9014 CG2 ILE E 482 61.675 42.574 36.355 1.00 50.34 C ATOM 9015 CD1 ILE E 482 63.635 38.800 39.991 1.00 47.59 ATOM 9016 N THR E 483 63.789 38.092 41.270 1.00 49.09 C ATOM 9017 CA THR E 483 ATOM 9018 C THR E 483 65.261 37.914 41.614 1.00 50.39 C 65.722 38.227 42.715 1.00 51.42 0 ATOM 9019 O THR E 483 C 63.104 36.723 41.224 1.00 49.12 ATOM 9020 CB THR E 483 61.695 36.995 41.063 1.00 50.26 0 ATOM 9021 OG1 THR E 483 63.398 35.939 42.479 1.00 48.46 C ATOM 9022 CG2 THR E 483 66.058 37.432 40.643 1.00 50.79 N ATOM 9023 N ASP E 484 C 67,484 37.245 40.832 1.00 49.22 ATOM 9024 CA ASP E 484 68.094 38.564 41.260 1.00 48.29 C ATOM 9025 C ASP E 484 ATOM 9026 O ASP E 484 68.896 38.610 42.191 1.00 49.77 68.170 36.726 39.587 1.00 50.22 C ATOM 9027 CB ASP E 484 C 67.746 35.330 39.199 1.00 51.85 ATOM 9028 CG ASP E 484 0 67.187 34.618 40.058 1.00 52.04 ATOM 9029 OD1 ASP E 484 ATOM 9030 OD2 ASP E 484 67.976 34.955 38.012 1.00 53.07 0 N 67.724 39.671 40.648 1.00 47.30 ATOM 9031 N THR E 485 68,307 40.957 41.023 1.00 48.09 C ATOM 9032 CA THR E 485 68,041 41.258 42.493 1.00 50.40 С ATOM 9033 C THR E 485 68.888 41.782 43.230 1.00 50.86 0 ATOM 9034 O THR E 485 67.688 42.030 40.127 1.00 46.75 C ATOM 9035 CB THR E 485 67.890 41.599 38.792 1.00 46.68 0 ATOM 9036 OG1 THR E 485 68.324 43.380 40.335 1.00 46.98 C ATOM 9037 CG2 THR E 485 66.818 40.925 42.940 1.00 50.66 N ATOM 9038 N LEUE 486 66.450 41.162 44.319 1.00 50.23 C ATOM 9039 CA LEU E 486 C 67.342 40.380 45.273 1.00 51.60 ATOM 9040 C LEUE 486 67.909 40.953 46.218 1.00 52.24 ATOM 9041 O LEUE 486 C 64.991 40.763 44.550 1.00 47.97 ATOM 9042 CB LEU E 486 64.025 41.941 44.459 1.00 47.38 C ATOM 9043 CG LEU E 486 62.620 41.409 44.670 1.00 46.61 C ATOM 9044 CD1 LEU E 486 C 64.395 43.072 45.410 1.00 46.32 ATOM 9045 CD2 LEU E 486 67.454 39.076 45.010 1.00 52.13 N ATOM 9046 N ILE E 487 ATOM 9047 CA ILE E 487 68.281 38.236 45.869 1.00 53.81 C 69.715 38.753 45.883 1.00 55.54 C ATOM 9048 C ILE E 487 ATOM 9049 O ILEE 487 70.364 38.863 46.912 1.00 55.11 0 ATOM 9050 CB ILE E 487 68.282 36.788 45.368 1.00 53.59 C

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ATOM	9145 CA GLN E 500	67.226 36.271 51.869 1.00 61.30 65.864 35.705 51.472 1.00 59.52	С
ATOM	9146 C GLN E 500	65.864 35.705 51.472 1.00 59.52	С
ATOM	9147 O GLN E 500	64.999 36.518 51.111 1.00 59.50	0
ATOM	9148 CB GLN E 500	68.304 35.728 50.970 1.00 62.53	С
ATOM	9149 CG GLN E 500	69.567 36.574 50.69 1.00 63.94 70.657 35.694 50.265 1.00 64.75	С
ATOM	9150 CD GLN E 500	70.657 35.694 50.265 1.00 64.75	С
ATOM	9151 OE1 GLN E 500	70.508 35.048 49.230 1.00 64.72	0
ATOM	9152 NE2 GLN E 500	71.778 35.663 50.965 1.00 66.02	N
		65.646 34.385 51.568 1.00 56.28	
		64.327 33.904 51.165 1.00 54.76	
ATOM	9155 C HISE 501	63.212 34.489 52.015 1.00 54.80	
ATOM	9156 O HIS E 501	62.118 34.664 51.456 1.00 56.59	0_
ATOM	9157 CB HIS E 501	64.183 32.405 51.063 1.00 54.63	С
		64.301 31.550 52.271 0.50 53.86	
ATOM	9159 CG BHIS E 501	65.370 31.733 50.443 0.50 55.35	C
ATOM	9160 NDIAMS E 501	05.085 30.406 52.291 0.50 53.73	N
ATOM	O162 CD2ALTS E 501	65.085 30.406 52.291 0.50 53.73 65.831 32.076 49.196 0.50 55.39 63.744 31.631 53.495 0.50 53.43	IN C
ATOM	0162 CD2AM3 E 301	66.186 30.756 50.904 0.50 55.24	C
ATOM	9103 CD2BHI3 E 501	65 005 20 827 52 476 0 50 52 22	C
ATOM	0165 CEIRHIS E 501	65.005 29.837 53.476 0.50 53.33 66.886 31.338 48.908 0.50 55.63 64.196 30.564 54.223 0.50 53.32	C
ATOM	9166 NF2AHTS F 501	64 196 30 564 54 223 0 50 53 32	N
ATOM	9167 NE2BHIS E 501	67.120 30.534 49.931 0.50 55.54	N
		63.388 34.815 53.283 1.00 52.93	
ATOM	9169 CA GLN E 502	62.318 35.390 54.078 1.00 51.36	C
ATOM	9170 C GLN E 502	62.318 35.390 54.078 1.00 51.36 61.987 36.780 53.587 1.00 50.30	C
		60.831 37.091 53.311 1.00 49.64	
ATOM	9172 CB GLN E 502	62.717 35.357 55.551 1.00 52.69	С
ATOM	9173 CG GLN E 502	62.955 33.916 55.981 1.00 54.06 62.980 33.648 57.462 1.00 54.41	С
<b>ATOM</b>	9174 CD GLN E 502	62.980 33.648 57.462 1.00 54.41	С
ATOM	9175 OE1 GLN E 502	63.315 34.510 58.275 1.00 55.01	0
	9176 NE2 GLN E 502		N
	9177 N ARG E 503	62.974 37.649 53.412 1.00 49.44	N
	9178 CA ARG E 503	62.730 38.998 52.915 1.00 47.48	C
	9179 C ARGE 503	62.002 38.993 51.577 1.00 47.83	C
	9180 O ARGE 503	61.044 39.720 51.335 1.00 48.42	0
	9181 CB ARGE 503	64.039 39.753 52.713 1.00 45.77	C
	9182 CG ARGE 503	63.784 41.259 52.699 1.00 45.18	C
	9183 CD ARGE 503	65.074 42.045 52.865 1.00 44.12	C
	9184 NE ARGE 503		N C
	9185 CZ ARGE 503		C
	9186 NH1 ARG E 503 9187 NH2 ARG E 503		N N
	9187 NH2 ARG E 303 9188 N LEU E 504	62.456 38.159 50.638 1.00 47.24	N
	9189 CA LEUE 504	61.835 38.066 49.334 1.00 45.05	C
ATOM	9109 CA LEU E 304	01.03 30.00 45.54 1.00 43.03	C

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ATOM	9325 ND2 ASN F 519	41.782 44.115 43.392 1.00 46.73	N
		40.259 48.867 45.721 1.00 45.70	
		39.382 49.814 46.402 1.00 46.05	
ATOM	9328 C LYS E 520	39.572 51.228 45.860 1.00 45.58	
ATOM	9329 O LYS E 520	39.572 51.228 45.860 1.00 45.58 38.594 51.950 45.722 1.00 45.26	O
		39.722 49.816 47.888 1.00 48.01	
ATOM	9331 CG LYS E 520	40.001 48.371 48.311 1.00 50.52	С
<b>ATOM</b>	9332 CD LYS E 520	38.723 47.900 48.965 1.00 54.26	С
ATOM	9333 CE LYS E 520	38.044 46.761 48.220 1.00 56.67	С
		36.608 46.682 48.688 1.00 58.30	
ATOM	9335 N GLY E 521	40.808 51.632 45.554 1.00 44.85	N
<b>ATOM</b>	9336 CA GLY E 521	41.030 52.952 45.003 1.00 45.03	C
		40.250 53.175 43.705 1.00 45.77	
		39.647 54.264 43.636 1.00 45.70	
		40.225 52.273 42.702 1.00 45.27	
		39.478 52.571 41.511 1.00 45.39	
		37.991 52.603 41.872 1.00 47.59	
		37.272 53.433 41.349 1.00 48.56	
ATOM	9343 CB MET E 522	39.441 51.667 40.334 1.00 45.90	C
ATOM	9344 CG MET E 522	40.441 50.747 39.785 1.00 47.11 41.710 51.489 38.776 1.00 48.25	C
ATOM	9345 SD MET E 522	41.710 51.489 38.776 1.00 48.25	S
		40.843 52.867 38.058 1.00 46.66	
		37.544 51.681 42.724 1.00 49.63	
		36.130 51.710 43.074 1.00 50.27	
		35.820 53.102 43.575 1.00 47.33	
		34.871 53.689 43.113 1.00 48.01 35.797 50.628 44.069 1.00 56.25	
ATOM	9331 CB GLUE 323	35.797 30.028 44,009 1,00 30.23	C C
ATOM	9332 CO GLUE 323	35.392 49.313 43.452 1.00 63.89 34.322 49.449 42.383 1.00 69.24	C
ATOM	9353 CD GLUE 323	33.579 50.482 42.394 1.00 72.11	0
		34.219 48.511 41.541 1.00 71.58	
		36.596 53.689 44.450 1.00 44.84	N
		36.385 55.020 44.954 1.00 44.01	Ċ
			c
	9359 O HIS E 524	35.654 57.015 43.827 1.00 43.85	O
		37.437 55.270 46.046 1.00 43.01	C
	9361 CG HIS E 524	37.353 56.633 46.640 1.00 42.25	С
<b>ATOM</b>	9362 ND1 HIS E 524	38.045 57.704 46.130 1.00 43.08	N
<b>ATOM</b>	9363 CD2 HIS E 524	36.678 57.129 47.680 1.00 42.58	C
<b>ATOM</b>	9364 CE1 HIS E 524	37.801 58.793 46.823 1.00 43.17	С
ATOM	9365 NE2 HIS E 524	36.960 58.463 47.792 1.00 42.97	N
ATOM	9366 N LEUE 525	37.559 56.112 43.109 1.00 46.94	N
ATOM	9367 CA LEU E 525	37.779 57.153 42.110 1.00 49.17	С
ATOM	9368 C LEUE 525	36.580 57.212 41.165 1.00 52.01	С
ATOM	9369 O LEUE 525	36.148 58.223 40.631 1.00 52.24	Ο

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ATOM	9415 SG BCYS E 530	28.141 57.575 38.467 0.50 79.92	S
ATOM	9416 N LYS E 531	29.719 61.034 41.209 1.00 81.60	N
ATOM	9417 CA LYS E 531	29.214 62.129 42.002 1.00 83.48	С
ATOM	9418 C LYS E 531	29.595 63.461 41.359 1.00 84.84	С
ATOM	9419 O LYS E 531	29.278 64.547 41.844 1.00 85.98	0
ATOM	9420 CB LYS E 531	29.842 62.116 43.398 1.00 84.16	С
ATOM	9421 CG LYS E 531	29.174 61.255 44.438 1.00 85.42	С
<b>ATOM</b>	9422 CD LYS E 531	28.963 59.818 43.955 1.00 86.01	С
<b>ATOM</b>	9425 N ASN E 532	30.319 63.462 40.270 1.00 86.16	N
<b>ATOM</b>	9426 CA ASN E 532	30.755 64.643 39.563 1.00 87.97	С
<b>ATOM</b>	9427 C ASN E 532	31.574 65.543 40.461 1.00 86.77	С
<b>ATOM</b>	9428 O ASN E 532	31.222 66.693 40.662 1.00 88.13	0
<b>ATOM</b>	9429 CB ASN E 532	29.554 65.398 38.999 1.00 91.01	С
<b>ATOM</b>	9430 CG ASN E 532	28.912 64.605 37.876 1.00 94.27	С
<b>ATOM</b>	9431 OD1 ASN E 532	29.637 64.076 37.022 1.00 95.71	0
<b>ATOM</b>	9432 ND2 ASN E 532	27.576 64.537 37.908 1.00 95.97	N
ATOM	9433 N VALE 533	32.655 65.054 41.021 1.00 85.06	N
ATOM	9434 CA VALE 533	33.541 65.790 41.909 1.00 83.95	С
ATOM	9435 C VAL E 533	34.955 65.844 41.319 1.00 83.81	С
ATOM	9436 O VAL E 533	35.866 66.622 41.603 1.00 84.30	Ο
		33.629 65.021 43.246 1.00 83.54	С
		34.400 65.798 44.283 1.00 83.03	С
ATOM	9439 CG2 VAL E 533	32.267 64.604 43.766 1.00 83.52	С
ATOM	9440 N VAL E 534	35.204 64.903 40.422 1.00 82.89	N
ATOM	9441 CA VALE 534	36.458 64.700 39.731 1.00 82.04	, C
ATOM			С
ATOM	9443 O VAL E 534	35.475 65.259 37.609 1.00 80.09	Ο
		36.672 63.185 39.430 1.00 82.66	С
		37.826 62.837 38.501 1.00 81.66	С
		36.855 62.411 40.735 1.00 83.03	С
	9447 N PRO E 535		N
ATOM		37.652 66.898 36.924 1.00 81.29	С
ATOM	9449 C PRO E 535	37.861 65.887 35.797 1.00 82.66	С
		38.163 64.695 35.919 1.00 82.39	0
	9451 CB PRO E 535		С
		39.350 67.541 38.473 1.00 79.86	С
		38.586 66.375 39.054 1.00 80.52	С
	9454 N LEUE 536	37.723 66.431 34.588 1.00 84.27	N
	9455 CA LEUE 536	37.837 65.722 33.337 1.00 84.25	С
	9456 C LEUE 536	39.244 65.558 32.805 1.00 83.95	C
	9457 O LEUE 536	39.442 65.872 31.616 1.00 85.68	0
		40.179 65.068 33.627 1.00 81.54	N
	9463 CA TYR E 537	41.537 64.848 33.115 1.00 78.07	C
	9464 C TYR E 537		C
ATOM	9465 O TYR E 537	40.988 62.554 32.656 1.00 74.94	0

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ATOM	9511 CG GLUE 542	42.968 56.080 28.183 1.00 55.43	С
ATOM	9512 CD GLU E 542	44.007 56.740 27.278 1.00 56.20	C
ATOM	9513 OE1 GLU E 542	43.863 57.973 27.045 1.00 56.53	0
ATOM	9514 OE2 GLU E 542	44.915 56.000 26.861 1.00 56.06	Ο
		42.772 55.618 31.884 1.00 50.13	
		43.183 54.486 32.707 1.00 50.01	
		42.037 53.999 33.574 1.00 50.73	
ATOM	9518 O MET E 543	41.896 52.801 33.859 1.00 51.88	0
ATOM	9519 CB MET E 543	44.387 54.921 33.546 1.00 50.17 45.472 55.536 32.658 1.00 50.14	C
ATOM	9520 CG MET E 543	45.472 55.536 32.658 1.00 50.14 46.371 54.190 31.854 1.00 49.83	C S
		46.371 34.190 31.834 1.00 49.83	
ATOM	9522 CL MET L 545	41 160 54 898 34 041 1 00 50 39	N
ATOM	9524 CA LEUE 544	41.169 54.898 34.041 1.00 50.39 40.056 54.453 34.866 1.00 51.08	C
ATOM	9525 C LEUE 544	39.119 53.599 34.022 1.00 52.64	C
ATOM	9526 O LEUE 544	38.687 52.545 34.503 1.00 51.89	0
ATOM	9527 CB LEUE 544	39.336 55.621 35.501 1.00 49.82	С
ATOM	9528 CG LEU E 544	39.336 55.621 35.501 1.00 49.82 38.032 55.374 36.237 1.00 49.45	С
ATOM	9529 CD1 LEU E 544	38.119 54.490 37.461 1.00 48.18	С
		37.470 56.718 36.684 1.00 50.84	
ATOM	9531 N ASP E 545	38.832 54.032 32.797 1.00 55.61	N
ATOM	9532 CA ASP E 545	37.941 53.268 31.941 1.00 59.73 38.457 51.892 31.603 1.00 59.61	С
ATOM	9533 C ASP E 545	38.457 51.892 31.603 1.00 59.61	C
ATOM	9534 O ASP E 545	37.635 50.985 31.534 1.00 60.30	0
ATOM	9333 CB ASP E 343	37.564 53.923 30.628 1.00 64.39	C
ATOM	9330 CO ASP E 343	36.754 55.196 30.851 1.00 69.96 36.217 55.451 31.975 1.00 71.84	0
ATOM	9538 OD2 ASP F 545	36.660 55.974 29.843 1.00 72.34	0
		39.748 51.701 31.435 1.00 60.47	
		40.297 50.385 31.144 1.00 61.70	
	9541 C ALA E 546		C
	9542 O ALA E 546	39.329 48.283 31.712 1.00 63.79	0
		41.803 50.399 31.291 1.00 61.61	С
	9544 N HIS E 547	39.719 49.673 33.392 1.00 66.30	N
	9545 CA HIS E 547	39.225 48.863 34.455 1.00 69.24	C
	9546 C HIS E 547	37.740 48.630 34.433 1.00 73.60	С
	9547 O HIS E 547	37.308 47.495 34.626 1.00 75.89	0
	9548 CB HIS E 547	39.532 49.620 35.773 1.00 67.78	C C
	9549 CG HIS E 547 9550 ND1 HIS E 547	40.989 49.285 35.946 1.00 66.33 41.415 48.311 36.802 1.00 66.23	N
	9551 CD2 HIS E 547	42.059 49.802 35.319 1.00 65.84	C
	9552 CEI HIS E 547	42.729 48.249 36.709 1.00 66.64	C
	9553 NE2 HIS E 547	43.144 49.133 35.819 1.00 66.16	N
	9554 N ARG E 548	36.961 49.670 34.230 1.00 78.65	N
	9555 CA ARG E 548	35.501 49.450 34.225 1.00 83.82	С

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ATOM 9556 C ARG E 548		С
ATOM 9557 O ARGE 548		Ō
	34.801 50.810 34.241 1.00 87.54	С
ATOM 9559 CG ARG E 548	35.485 51.952 34.980 1.00 90.41	С
ATOM 9560 CD ARG E 548	35.811 51.738 36.443 1.00 93.01	С
ATOM 9561 NE ARG E 548	35.074 50.727 37.193 1.00 95.25	N
	35.442 50.146 38.337 1.00 96.28	С
	36.575 50.450 38.957 1.00 96.79	
	34.660 49.227 38.903 1.00 96.67	N
TER 9565 ARG E 548		_
HETATM 9566 C1 EST E 600	47.222 60.396 43.519 1.00 34.93	С
HETATM 9567 C2 EST E 600	48.571 60.475 43.210 1.00 37.57	C
HETATM 9568 C3 EST E 600	49.436 59.518 43.657 1.00 38.54	C
HETATM 9569 O3 EST E 600 HETATM 9570 C4 EST E 600	50.769 59.635 43.327 1.00 40.09 49.033 58.426 44.443 1.00 37.89	O C
HETATM 9570 C4 EST E 600 HETATM 9571 C5 EST E 600	47.646 58.348 44.751 1.00 36.69	C
HETATM 9571 C5 EST E 600 HETATM 9572 C6 EST E 600		
HETATM 9573 C7 EST E 600		
HETATM 9574 C8 EST E 600		č
HETATM 9575 C9 EST E 600	45.317 59.266 44.607 1.00 33.78	Č
HETATM 9576 C10 EST E 600		С
HETATM 9577 C11 EST E 600		С
HETATM 9578 C12 EST E 600	42.980 59.847 43.918 1.00 34.32	
HETATM 9579 C13 EST E 600	42.578 58.437 44.347 1.00 34.56	С
HETATM 9580 C14 EST E 600		C
HETATM 9581 C15 EST E 600		
HETATM 9582 C16 EST E 600		
HETATM 9583 C17 EST E 600		
HETATM 9584 O17 EST E 600		O C
HETATM 9585 C18 EST E 600 ATOM 9586 N SER F 305	42.511 57.536 43.119 1.00 34.18 54.849 29.184 70.902 1.00 88.75	N
ATOM 9587 CA SER F 305	53.873 28.738 69.869 1.00 88.59	C
ATOM 9587 CA SER F 305	54.304 27.466 69.171 1.00 87.91	c
ATOM 9589 O SER F 305	55.423 27.412 68.680 1.00 87.92	Ö
	53.698 29.871 68.839 1.00 88.47	C
ATOM 9591 OG SER F 305	52.794 29.522 67.815 1.00 88.14	O
ATOM 9592 N LEUF 306	53.428 26.475 69.068 1.00 87.84	N
ATOM 9593 CA LEUF 306	53.764 25.236 68.354 1.00 87.46	С
ATOM 9594 C LEU F 306	54.314 25.700 67.008 1.00 86.18	С
ATOM 9595 O LEUF 306	55.444 25.390 66.663 1.00 86.66	0
ATOM 9596 CB LEUF 306	52.565 24.313 68.117 1.00 88.10	C
ATOM 9600 N ALA F 307	53.519 26.485 66.291 1.00 84.32	N
ATOM 9601 CA ALA F 307	53.906 27.037 65.014 1.00 82.77	C
ATOM 9602 C ALA F 307	55.411 27.233 64.958 1.00 81.44	C
ATOM 9603 O ALA F 307	56.089 26.580 64.173 1.00 81.34	J

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ATOM	9604 CB ALA F 307	53.245 28.399 64.801 1.00 83.53	С
ATOM	9605 N LEUF 308	55.926 28.106 65.806 1.00 80.43	N
		57.349 28.379 65.823 1.00 80.87	С
	9607 C LEUF 308		С
	9608 O LEUF 308		Ο
		57.544 29.609 66.728 1.00 80.50	С
		56.845 30.879 66.264 1.00 80.59	С
		57.464 32.127 66.851 1.00 80.80	С
	9612 CD2 LEU F 308		С
	9613 N SER F 309		N
	9614 CA SER F 309	58.715 24.939 66.908 1.00 79.92	С
	9615 C SER F 309		C
	9616 O SER F 309		0_
		58.114 24.299 68.174 1.00 81.24	C
		57.899 25.422 69.018 1.00 85.04	0
		57.616 23.617 65.203 1.00 76.56	N
		57.582 22.522 64.249 1.00 73.92	C
	9621 C LEUF 310		C
	9622 O LEUF 310		0
		56.234 22.376 63.594 1.00 73.55 55.028 22.755 64.432 1.00 72.82	С
			C
		54.354 23.914 63.716 1.00 73.19 54.108 21.571 64.611 1.00 73.65	C C
		59.062 21.572 62.657 1.00 71.49	N
		60.116 21.538 61.647 1.00 71.49	C
ATOM	9629 C. THR F 311	59.429 21.644 60.311 1.00 70.16	c
	9630 O THR F 311		ŏ
		60.900 20.230 61.811 1.00 71.14	C
		60.069 19.092 61.584 1.00 70.69	O
ATOM	9633 CG2 THR F 311	61.389 20.113 63.250 1.00 71.71	Č
	9634 N ALA F 312		N
	9635 CA ALA F 312	59.383 22.153 57.967 1.00 69.06	C
	9636 C ALA F 312	58.565 20.893 57.733 1.00 69.29	C
	9637 O ALA F 312	57.430 20.985 57.256 1.00 69.18	O
<b>ATOM</b>	9638 CB ALA F 312	60.315 22.432 56.817 1.00 69.25	<b>C</b> .
ATOM	9639 N ASP F 313	59.097 19.728 58.054 1.00 70.53	N
<b>ATOM</b>	9640 CA ASP F 313	58.342 18.498 57.862 1.00 72.19	С
ATOM-	9641 C ASP F 313	57.094 18.407 58.701 1.00 70.29	С
ATOM	9642 O ASP F 313	56.062 18.015 58.167 1.00 69.40	0
	9643 CB ASP F 313	59.258 17.290 58.105 1.00 76.57	С
	9644 CG ASP F 313	60.094 17.159 56.828 1.00 80.64	C
	9645 OD1 ASP F 313	59.456 17.019 55.745 1.00 82.23	О
	9646 OD2 ASP F 313	61.339 17.234 56.980 1.00 82.58	0
	9647 N GLN F 314	57.138 18.766 59.970 1.00 69.39	N
ATOM	9648 CA GLN F 314	55.944 18.701 60.805 1.00 69.22	С

ATOM 9691 CA LEU F 320 48.275 18.289 55.072 1.00 58.32

51.064 24.328 56.054 1.00 49.82

48.990 24.419 57.502 1.00 49.44

48.861 19.348 55.901 1.00 56.35

47.143 17.594 55.799 1.00 61.15

46.190 17.106 55.215 1.00 61.84

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ATOM 9688 CD1 LEU F 319

ATOM 9689 CD2 LEU F 319

ATOM 9690 N LEUF 320

ATOM 9692 C LEUF 320

ATOM 9693 O LEUF 320

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9739 CG1 ILE F 326	35.729 15.472 48.160 1.00 66.76	С
		С
9741 CD1 ILE F 326		С
9742 N LEUF 327	33.286 18.514 49.471 1.00 59.83	N
		С
9744 C LEUF 327	31.345 17.922 48.116 1.00 60.14	С
	32.115 17.939 47.156 1.00 60.86	O
9746 CB LEUF 327	31.214 19.684 49.901 1.00 57.70	С
9747 CG LEUF 327	31.777 20.287 51.182 1.00 57.55	С
9748 CD1 LEU F 327	30.782 21.285 51.776 1.00 57.69	С
9749 CD2 LEU F 327	32.117 19.257 52.241 1.00 57.43	С
		N
	29.522 17.172 46.703 1.00 62.52	С
9752 C TYR F 328	28.386 18.181 46.541 1.00 63.58	С
		Ο
9754 CB TYR F 328		С
		С
		C
9757 CD2 TYR F 328	30.317 14.351 45.203 1.00 64.90	C
9758 CE1 TYR F 328	31.533 13.198 47.392 1.00 66.06	C
9759 CE2 TYR F 328		C
	_	C
		0
		N
		C
		C
		0
9766 CB SER F 329	27.102 20.126 43.683 1.00 68.03	C
		0
		N
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		C C
		0
		0
		N
		C
		C
		0
		C
		C
		C
9783 CD1 PHE F 337	22.817 24.805 36.239 1.00 87.30	C
	9740 CG2 ILE F 326 9741 CD1 ILE F 326 9742 N LEU F 327 9743 CA LEU F 327 9744 C LEU F 327 9745 O LEU F 327 9746 CB LEU F 327 9747 CG LEU F 327 9748 CD1 LEU F 327 9749 CD2 LEU F 327 9750 N TYR F 328 9751 CA TYR F 328 9751 CA TYR F 328 9753 O TYR F 328 9754 CB TYR F 328 9755 CG TYR F 328 9756 CD1 TYR F 328 9757 CD2 TYR F 328 9758 CE1 TYR F 328 9759 CE2 TYR F 328 9760 CZ TYR F 328 9760 CZ TYR F 328 9761 OH TYR F 328 9762 N SER F 329 9763 CA SER F 329 9764 C SER F 329 9765 O SER F 329 9766 CB SER F 329 9767 OG SER F 329 9768 N GLU F 330 9770 C GLU F 330 9770 C GLU F 330 9771 O GLU F 330 9771 O GLU F 330 9772 CB GLU F 330 9773 CG GLU F 330 9774 CD GLU F 330 9775 OE1 GLU F 330 9775 OE1 GLU F 330 9776 OE2 GLU F 330 9777 CPHE F 337 9778 CA PHE F 337 9778 CA PHE F 337	9739 CG1 ILE F 326 9740 CG2 ILE F 326 9741 CD1 ILE F 326 9742 N LEU F 327 9743 CA LEU F 327 9744 C LEU F 327 9745 O LEU F 327 9746 CB LEU F 327 9747 CG LEU F 327 9748 CD1 LEU F 327 9749 CD2 LEU F 327 9750 N TYR F 328 9751 CA TYR F 328 9752 C TYR F 328 9753 O TYR F 328 9755 CG TYR F 328 9755 CG TYR F 328 9756 CD1 TYR F 328 9756 CD1 TYR F 328 9757 CD2 TYR F 328 9758 CE1 TYR F 328 9759 CE2 TYR F 328 9750 C TYR F 328 9751 CA SER F 329 9760 CZ TYR F 328 9761 OH TYR F 328 9766 CB SER F 329 9766 CB SER F 329 9766 CB SER F 329 9767 OG SER F 329 9767 OG SER F 329 9768 N GLU F 330 9770 C GLU F 330 9771 O GLU F 330 9772 CB GLU F 330 9773 CG GLU F 330 9775 OEI GLU F 330 9776 OE2 GLU F 330 9777 N PHE F 337 9778 CA PHE F 337 9778 CB PHE F 337 9781 CB PHE F 337 9782 CB PHE F 337 9781 CB PHE F 337

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ATOM	9784 CD2 PHF F 337	24.095 24.380 34.276 1.00 87.89	С
ATOM	9785 CE1 PHE F 337	23.642 23.957 36.942 1.00 88.83	Č
		24.929 23.526 34.962 1.00 88.18	
ATOM	9787 CZ PHE F 337	24.698 23.318 36.308 1.00 89.08	С
ATOM	9788 N SER F 338	20.037 28.218 35.270 1.00 80.62	N
		19.577 29.573 34.995 1.00 78.22	
		20.401 30.467 35.897 1.00 76.60	
ATOM	9/91 O SER F 338	20.845 29.967 36.939 1.00 76.99	0
ATOM	9/92 CB SER F 338	18.088 29.667 35.311 1.00 78.08 17.785 29.015 36.523 1.00 77.58	C O
ATOM	9794 N GLUF 339	20.575 31.736 35.600 1.00 74.82	N
		21.318 32.604 36.534 1.00 73.09	
ATOM	9796 C GLU F 339	20 939 32 174 37 951 1 00 71 30	C
ATOM	9797 O GLU F 339	21.769 31.721 38.735 1.00 70.30	0
		20.958 34.040 36.203 1.00 73.57	
		21.102 35.120 37.254 1.00 74.18	
ATOM	9800 CD GLUF 339	21.495 36.392 36.517 1.00 75.77	C
ATOM	9801 OE1 GLUF 339	22.483 36.313 35.744 1.00 75.89	0
		20.817 37.433 36.705 1.00 77.28 19.648 32.249 38.293 1.00 69.59	
		19.192 31.861 39.607 1.00 67.96	
ATOM	9805 C ALA F 340	19.566 30.438 39.970 1.00 66.96	c
		20.091 30.235 41.066 1.00 68.75	
		17.687 32.024 39.737 1.00 67.62	
ATOM	9808 N SER F 341	19.302 29.459 39.142 1.00 65.15	N
ATOM	9809 CA SER F 341	19.618 28.088 39.529 1.00 65.19	С
		21.108 27.902 39.705 1.00 63.98	
		21.522 27.252 40.673 1.00 64.74 19.004 27.077 38.566 1.00 67.22	
ATOM	9813 OG SER F 341	19.940 26.356 37.790 1.00 69.32	0
	9814 N MET F 342		N
		23.380 28.262 38.976 1.00 60.83	C
ATOM	9816 C MET F 342	23.917 28.994 40.201 1.00 59.89	С
	9817 O MET F 342	24.616 28.406 41.027 1.00 60.05	0
	9818 CB MET F 342	24.168 28.719 37.751 1.00 60.66	C
	9819 CG MET F 342	25.596 28.200 37.887 1.00 61.87	C
	9820 SD MET F 342 9821 CE MET F 342	26.497 28.176 36.308 1.00 63.51 26.629 29.935 36.028 1.00 62.32	S C
	9822 N MET F 343	23.563 30.272 40.396 1.00 58.10	N
	9823 CA MET F 343	24.029 31.011 41.555 1.00 56.16	C
	9824 C MET F 343	23.676 30.186 42.780 1.00 56.22	c
	9825 O MET F 343	24.486 30.013 43.683 1.00 57.06	Ō
	9826 CB MET F 343	23.404 32.383 41.634 1.00 56.11	С
		24.093 33.365 40.708 1.00 56.34	C
ATOM	9828 SD MET F 343	25.845 33.433 41.051 1.00 56.93	S

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9829	CE MET F 343		C
9830	N GLY F 344	22.460 29.655 42.797 1.00 55.26	N
9831	CA GLY F 344	22.027 28.824 43.901 1.00 54.47	С
9832	C GLY F 344	23.031 27.729 44.216 1.00 53.83	С
9833	O GLY F 344	23.477 27.716 45.366 1.00 53.45	0
9834	N LEUF 345	23.372 26.851 43.267 1.00 53.87	N
9835	CA LEUF 345	24.314 25.771 43.552 1.00 53.39	С
9836	C LEUF 345	25.656 26.242 44.104 1.00 52.00	С
9837	O LEUF 345	26.099 25.789 45.146 1.00 51.76	0
9838	CB LEUF 345	24.739 25.014 42.299 1.00 54.69	С
			С
9840	CD1 LEU F 345	23.450 24.634 40.246 1.00 57.95	С
9841	CD2 LEU F 345	24.072 22.682 41.765 1.00 57.27	С
9842	N LEU F 346	26.249 27.134 43.309 1.00 49.99	N
9843	CA LEUF 346		C
			С
			Ο
			С
			С
			С
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			N
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			C
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			0
			N
			N
			C
			С
			0
			C C
			C C
	*		N
9873	N ALAF33U	29.343 27.020 48.400 1.00 41.32	14
	9830 9831 9832 9833 9834 9835 9836 9837 9840 9841 9842 9843 9844 9845 9847 9848 9849 9850 9851 9852 9853 9854 9855 9857 9858 9859 9860 9861 9862 9863 9864 9865 9866 9867 9870 9871 9872	9830 N GLY F 344 9831 CA GLY F 344 9832 C GLY F 344 9833 O GLY F 344 9834 N LEU F 345 9835 CA LEU F 345 9836 C LEU F 345 9837 O LEU F 345 9839 CG LEU F 345 9840 CD1 LEU F 345 9841 CD2 LEU F 346 9842 N LEU F 346 9843 CA LEU F 346 9844 C LEU F 346 9845 O LEU F 346 9846 CB LEU F 346 9847 CG LEU F 346 9848 CD1 LEU F 346 9849 CD2 LEU F 346 9849 CD2 LEU F 346 9850 N THR F 347 9851 CA THR F 347 9851 CA THR F 347 9852 C THR F 347 9854 CB THR F 347 9855 OG1 THR F 347 9855 OG1 THR F 347 9856 CG2 THR F 347 9857 N ASN F 348 9859 C ASN F 348 9860 O ASN F 348 9861 CB ASN F 348 9861 CB ASN F 348 9863 OD1 ASN F 348 9864 ND2 ASN F 348 9865 N LEU F 349 9866 CA LEU F 349 9866 CA LEU F 349 9867 C LEU F 349 9869 CB LEU F 349	9831 CA GLY F 344 9832 C GLY F 344 9833 O GLY F 344 23.031 27.729 44.216 1.00 53.83 9834 N LEU F 345 9836 CA LEU F 345 9836 C LEU F 345 9837 O LEU F 345 9839 CG LEU F 345 9839 CG LEU F 345 9840 CD1 LEU F 345 9840 CD1 LEU F 345 9841 CD2 LEU F 345 9842 N LEU F 346 9843 CA LEU F 346 9844 C LEU F 346 9845 O LEU F 346 9846 CB LEU F 346 9847 CG LEU F 346 9848 CD1 LEU F 346 9849 CD2 LEU F 346 9848 CD1 LEU F 346 9849 CD2 LEU F 346 9849 CD2 LEU F 346 9847 CG LEU F 346 9848 CD1 LEU F 346 9849 CD2 LEU F 346 9849 CD2 LEU F 346 9850 N THR F 347 9851 CA THR F 347 9851 CA THR F 347 9855 CG THR F 347 9855 CG THR F 347 9856 CG Z THR F 347 9857 N ASN F 348 9858 CA ASN F 348 9860 O ASN F 348 9860 O ASN F 348 9860 O ASN F 348 9861 CB ASN F 348 9866 CA LEU F 349 9867 C LEU F 349 9870 CG LEU F 349 9871 CD1 LEU F 349 9872 CD2 LEU F 349 9877 CD1 LEU F 349 9877 CD2 LEU F 349 9878 CD2 LEU F 349 9879 CD2 LEU F 349 9879 CD2 LEU F 349 9877 CD2 LEU F 349 9877 CD2 LEU F 349 9878 CD2 LEU F 349 9879 CD2 LEU F 349 9879 CD2 LEU F 349 9879 CD2 LEU F 349 9877 CD2 LEU F 349 9877 CD2 LEU F 349 9878 CD3 LEU F 349 9879 CD2 LEU F 349 9879 CD2 LEU F 349 9877 CD2 LEU F 349

30.509 24.682 57.890 1.00 41.67

C

ATOM 9918 CB VAL F 355

			5 27 ( 3 × )	
ATOM	9919	CG1 VAL F 355	30.568 23.938 59.191 1.00 40.99	С
			29.276 25.541 57.764 1.00 42.17	С
ATOM			33,363 24,019 56,985 1.00 43.95	N
<b>ATOM</b>	9922	CA HISF356	34.607 23.267 57.066 1.00 45.14	С
<b>ATOM</b>	9923	C HIS F 356	35.765 24.222 57.213 1.00 44.30	С
<b>ATOM</b>	9924	O HIS F 356	36.682 24.016 58.008 1.00 44.09	0
<b>ATOM</b>	9925	CB HIS F 356	34.690 22.340 55.844 1.00 48.01	С
ATOM		CG HIS F 356	33.569 21.342 55.974 1.00 51.72	С
			33.751 20.044 56.403 1.00 53.60	N
			32.240 21.467 55.770 1.00 53.10	С
<b>ATOM</b>	9929	CE1 HIS F 356	32.580 19.434 56.435 1.00 53.89	С
<b>ATOM</b>		NE2 HIS F 356	31.634 20.265 56.056 1.00 53.29	N
ATOM		N MET F 357		N
ATOM		CA MET F 357		С
		C MET F 357		С
		O MET F 357		О
			36.486 27.554 55.656 1.00 42.86	C
			37.813 28.308 55.484 1.00 42.98	C
ATOM	9937	SD MET F 357	37.574 29.868 54.643 1.00 43.25	S
			37.137 29.259 52.991 1.00 43.78	С
		N ILEF358		N
			36.371 27.608 59.972 1.00 41.23	C
		C ILEF358		C
		O ILEF358	38.079 26.929 61.491 1.00 43.00	0
			35.003 27.877 60.634 1.00 39.57	C
			34.325 28.975 59.814 1.00 39.81	C
			35.123 28.255 62.078 1.00 37.70	C
			32.999 29.421 60.382 1.00 41.24	C
		N ASN F 359		N
			37.375 24.250 61.394 1.00 47.81	C
ATOM	9949	C ASN F 359	38.826 24.158 60.963 1.00 46.61	C
ATOM	9950	O ASN F 359	39.730 24.197 61.801 1.00 47.89	0
		CB ASN F 359		C
		CG ASN F 359	35.426 22.863 61.893 1.00 56.61	C
		OD1 ASN F 359	35.709 22.917 63.097 1.00 60.88	N
		ND2 ASN F 359	34.216 22.808 61.385 1.00 57.37 39.023 24.078 59.653 1.00 43.52	N
		N TRP F 360 CA TRP F 360	40.373 24.013 59.131 1.00 42.62	C
		C TRP F 360	41.264 25.111 59.670 1.00 42.88	c
		O TRP F 360	42.406 24.935 60.061 1.00 42.92	ŏ
		CB TRP F 360	40.226 24.186 57.614 1.00 42.66	C
		CG TRP F 360	41.553 24.512 57.001 1.00 42.12	Č
		CD1 TRP F 360	42.551 23.635 56.778 1.00 41.75	C
		CD2 TRP F 360	41.999 25.803 56.561 1.00 42.44	Č
		NEI TRP F 360	43.590 24.317 56.218 1.00 43.62	N
ATOM	7703	MELIKE F 300	73.330 27.317 30.216 1.00 73.02	14

wo	98/56812	330/371	PCT/GB98/01708
ATOM	9964 CE2 TRP F 360	43.299 25.645 56.061 1.00 42.40	С
		41.419 27.082 56.547 1.00 42.27	
	9966 CZ2 TRP F 360		
ATOM	9967 CZ3 TRP F 360	42.177 28.116 56.036 1.00 42.74	С
<b>ATOM</b>	9968 CH2 TRP F 360	43.478 27.906 55.548 1.00 42.73	С
		40.770 26.351 59.666 1.00 44.32	N
		41.496 27.515 60.143 1.00 44.21	С
		42.042 27.224 61.523 1.00 45.40	С
		43.218 27.491 61.736 1.00 45.18	0
		40.612 28.740 60.157 1.00 43.35	
	9974 N LYS F 362		N
		41.695 26.383 63.771 1.00 50.51	C
	9976 C LYS F 362	42.934 25.524 63.877 1.00 50.52 43.657 25.648 64.864 1.00 50.40	C 0
ATOM	9977 O LIST 302	40.524 25.801 64.571 1.00 53.28	C
		39.434 26.852 64.802 1.00 56.10	C
		39.915 27.861 65.822 1.00 58.93	
		38.881 28.178 66.898 1.00.61.09	
		39.409 29.008 68.036 1.00 61.11	
		43.241 24.677 62.936 1.00 50.76	
		44.398 23.836 62.900 1.00 52.41	
		45.589 24.400 62.149 1.00 51.42	С
		46.595 23.700 62.027 1.00 52.42	0
		44.027 22.559 62.132 1.00 57.14	
		42.522 22.408 62.005 1.00 63.12	
ATOM	9989 CD ARG F 363	42.037 21.691 63.293 1.00 69.42	С
		42.619 20.335 63.225 1.00 75.02	
		42.205 19.469 62.282 1.00 78.35	
		41.238 19.854 61.445 1.00 79.78 42.748 18.249 62.182 1.00 79.54	
	9994 N VALF 364		N
	9995 CA VAL F 364	46.754 26.080 60.871 1.00 47.95	C
	9996 C VAL F 364	47.689 26.535 61.964 1.00 47.06	C
	9997 O VAL F 364	47.364 27.425 62.733 1.00 47.62	0
<b>ATOM</b>	9998 CB VAL F 364	46.336 27.238 59.945 1.00 46.96	С
	9999 CG1 VAL F 364	47.520 27.990 59.395 1.00 46.14	С
	10000 CG2 VAL F 364	45.447 26.686 58.846 1.00 47.06	С
	10001 N PRO F 365	48.834 25.947 62.111 1.00 46.86	N
	10002 CA PRO F 365	49.795 26.303 63.142 1.00 47.30	С
	10003 C PRO F 365	49.914 27.803 63.280 1.00 47.97	C
	10004 O PRO F 365	50.102 28.494 62.282 1.00 49.63	0
_	10005 CB PRO F 365	51.119 25.617 62.755 1.00 46.66	C
	10006 CG PRO F 365 10007 CD PRO F 365	50.541 24.380 62.100 1.00 47.21 49.314 24.832 61.289 1.00 47.57	C C
	10007 CD PROF 365 10008 N GLY F 366	49.314 24.832 61.289 1.00 47.37 49.771 28.338 64.487 1.00 48.33	N
ATOM	10008 N GLIF300	47.771 20.330 04.467 1.00 40.33	14

			3511311	
			49.879 29.737 64.813 1.00 47.57	С
<b>ATOM</b>	10010	C GLY F 366	48.589 30.521 64.858 1.00 47.62	С
<b>ATOM</b>	10011	O GLY F 366	48.493 31.600 65.468 1.00 48.03	Ο
<b>ATOM</b>	10012	N PHE F 367	47.562 30.022 64.184 1.00 46.85	N
<b>ATOM</b>	10013	CA PHE F 367	46.281 30.718 64.081 1.00 46.59	С
<b>ATOM</b>	10014	C PHE F 367	45,595 30,997 65,410 1.00 46,36	С
<b>ATOM</b>	10015	O PHE F 367	45.152 32.047 65.848 1.00 45.52	0
<b>ATOM</b>	10016	CB PHE F 367	45.325 29.920 63.189 1.00 44.75	С
<b>ATOM</b>	10017	CG PHE F 367	44.071 30.654 62.850 1.00 44.60	С
ATOM	10018	CD1 PHE F 367	44.073 31.662 61.912 1.00 44.16	С
ATOM	10019	CD2 PHE F 367	42.875 30.334 63.491 1.00 45.67	С
			42.919 32.340 61.592 1.00 44.81	С
			41.696 30.997 63.180 1.00 45.38	С
			41.723 31.996 62.222 1.00 45.46	C
ATOM	10023	N VALF368	45.510 29.919 66.150 1.00 46.98	N
<b>ATOM</b>	10024	CA VAL F 368	44.884 29.809 67.454 1.00 47.50	С
<b>ATOM</b>	10025	C VAL F 368	45.555 30.694 68.470 1.00 48.39	С
<b>ATOM</b>	10026	O VAL F 368	44.887 31.054 69.446 1.00 49.08	Ο
<b>ATOM</b>	10027	CB VALF 368	44.845 28.309 67.816 1.00 46.46	С
<b>ATOM</b>	10028	CG1 VAL F 368	45.352 28.034 69.195 1.00 46.31	С
<b>ATOM</b>	10029	CG2 VAL F 368	43.434 27.799 67.573 1.00 46.30	С
<b>ATOM</b>	10030	N ASP F 369	46.810 31.080 68.264 1.00 48.91	N
<b>ATOM</b>	10031	CA ASP F 369	47.504 31.989 69.146 1.00 49.05	C
<b>ATOM</b>	10032	C ASP F 369	46.994 33.411 68.959 1.00 48.03	C
<b>ATOM</b>	10033	O ASP F 369	47.416 34.260 69.730 1.00 49.36	0
ATOM	10034	CB ASP F 369	49.005 32.039 68.908 1.00 52.31	C
<b>ATOM</b>	10035	CG ASP F 369	49.679 30.684 68.963 1.00 56.87	С
<b>ATOM</b>	10036	OD1 ASP F 369	49.349 29.868 69.872 1.00 59.10	О
<b>ATOM</b>	10037	OD2 ASP F 369	50.566 30.390 68.109 1.00 57.95	0
<b>ATOM</b>	10038	N LEU F 370	46.158 33.800 68.021 1.00 46.74	N
		CA LEUF 370	45.655 35.163 67.888 1.00 44.48	С
ATOM	10040	C LEU F 370	44.419 35.379 68.749 1.00 42.98	С
		O LEU F 370	43.795 34.398 69.161 1.00 42.49	0
		CB LEUF 370	45.321 35.373 66.403 1.00 45.02	С
		CG LEUF 370	46.514 35.297 65.452 1.00 45.13	C
_		CD1 LEU F 370	46.110 35.500 64.015 1.00 44.83	С
ATOM	10045	CD2 LEU F 370	47.506 36.398 65.830 1.00 45.41	С
		N THR F 371	44.016 36.601 69.059 1.00 41.35	N
		CA THR F 371	42.833 36.757 69.881 1.00 40.62	С
		C THR F 371	41.653 36.256 69.075 1.00 42.21	C
ATOM	10049	O THR F 371	41.627 36.260 67.864 1.00 42.62	Ο
		CB THR F 371	42.575 38.216 70.192 1.00 40.25	C
		OG1 THR F 371	42.670 38.876 68.928 1.00 42.32	0
		CG2 THR F 371	43.594 38.781 71.114 1.00 40.04	С
ATOM	10053	N LEUF 372	40.602 35.837 69.761 1.00 44.21	N

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ATOM 10054	CA LEUF 372	39.418 35.325 69.102 1.00 44.26	С
ATOM 10055	C LEUF 372	38.932 36.292 68.047 1.00 45.09	С
		38.550 35.821 66.966 1.00 46.27	
ATOM 10057	CB LEU F 372	38.388 35.012 70.186 1.00 43.22	С
ATOM 10058	CG LEUF 372	38.740 33.838 71.093 1.00 41.50	С
ATOM 10059	CD1 LEU F 372	38.740 33.838 71.093 1.00 41.50 37.680 33.752 72.173 1.00 42.51	С
ATOM 10060	CD2 LEU F 372	38.762 32.559 70.291 1.00 40.77	С
ATOM 10061	N HIS F 373	38.935 37.602 68.274 1.00 45.60	N
ATOM 10062	CA HIS F 373	38.399 38.491 67.238 1.00 46.42	С
ATOM 10063	C HIS F 373	39.328 38.508 66.059 1.00 45.56	С
		38.840 38.440 64.937 1.00 44.91	0
ATOM 10065	CB HIS F 373	38.048 39.845 67.807 1.00 49.57	С
ATOM 10066	CG HIS F 373	36.763 39.812 68.579 1.00 52.32	С
ATOM 10067	ND1 HIS F 373	36.676 39.816 69.958 1.00 53.50	· N
ATOM 10068	CD2 HIS F 373	35.497 39.767 68.163 1.00 53.33	C
ATOM 10069	CE1 HIS F 373	35.408 39.782 70.315 1.00 54.25	C
ATOM 10070	NE2 HIS F 373	35.408 39.782 70.315 1.00 54.25 34.653 39.741 69.241 1.00 54.69 40.637 38.530 66.279 1.00 45.43	N
ATOM 10071	N ASP F 374	40.637 38.530 66.279 1.00 45.43	N
ATOM 10072	CA ASP F 374	41.558 38.487 65.134 1.00 44.42	С
		41.355 37.269 64.272 1.00 43.20	
ATOM 10074	O ASP F 374	41.438 37.415 63.053 1.00 43.11	0
ATOM 10075	CB ASP F 374	43.004 38.647 65.603 1.00 45.47	C
		43.075 40.126 65.975 1.00 48.30	
		42.115 40.854 65.579 1.00 48.90	
		44.051 40.564 66.632 1.00 50.38	
		41.062 36.116 64.853 1.00 42.34	
		40.791 34.951 64.031 1.00 42.84	
		39.583 35.269 63.159 1.00 43.36	
ATOM 10082	CD CLN F 3/3	39.619 35.161 61.925 1.00 43.87	
ATOM 10083	CE CLN F 3/5	40.583 33.750 64.914 1.00 43.60	C C
	CD GLN F 375	41.827 33.439 65.729 1.00 45.60	C
	OE1 GLN F 375	41.568 32.352 66.757 1.00 46.87 40.780 31.422 66.560 1.00 47.29	0
	NE2 GLN F 375	42.244 32.497 67.888 1.00 47.07	N
	N VALF 376	38.496 35.752 63.774 1.00 43.02	N
	CA VALF 376	37.322 36.091 62.969 1.00 42.27	C
	C VAL F 376	37.749 37.033 61.861 1.00 42.22	č
	O VALF 376	37.412 36.808 60.705 1.00 43.67	Ö
	CB VALF 376	36.139 36.621 63.764 1.00 41.25	C
	CG1 VAL F 376	34.885 36.524 62.909 1.00 42.60	C
	CG2 VAL F 376	35.858 35.782 64.983 1.00 40.27	Č
	N HISF 377	38.514 38.062 62.146 1.00 42.99	N
	CA HISF 377	39.001 38.986 61.129 1.00 43.28	C
ATOM 10097	C HIS F 377	39.765 38.268 60.046 1.00 42.83	С
ATOM 10098	O HIS F 377	39.285 38.351 58.901 1.00 43.87	0

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		333/371	
	10099 CB HIS F 377		
		40.368 41.134 60.835 0.50 43.00	С
	10101 CG BHIS F 377		C
		39.590 42.070 60.187 0.50 43.19	
ATOM	10104 CD24FIS F 3//	38.930 41.315 63.832 0.50 45.60 41.632 41.377 60.432 0.50 43.03	N C
ATOM	10104 CD2AHIS F 377	41.632 41.377 60.432 0.50 43.02 37.684 41.620 62.069 0.50 45.70	C
ATOM	10106 CELAHIS F 377	40.346 42.832 59.421 0.50 42.88	Č
		37.937 42.103 64.205 0.50 45.09	
	10108 NE2AHIS F 377		
	10109 NE2BHIS F 377	37.168 42.296 63.156 0.50 45.46	
ATOM	10110 N LEUF 378	40.848 37.528 60.241 1.00 41.51	N
ATOM	10111 CA LEUF 378	41.470 36.883 59.064 1.00 40.44	С
<b>ATOM</b>	10112 C LEUF 378	40.465 36.050 58.284 1.00 39.92	C
ATOM	10113 O LEUF 378	40.382 36.020 57.037 1.00 38.68	0
_		42.724 36.129 59.482 1.00 41.23	С
		43.717 36.893 60.386 1.00 40.82	С
	10116 CD1 LEU F 378	44.893 36.008 60.747 1.00 40.06	C
	10117 CD2 LEU F 378		C
	10118 N LEUF 379		N
ATOM	10119 CA LEUF 3/9	38.587 34.518 58.288 1.00 39.44	C C
ATOM	10120 C LEUF 379	37.741 35.406 57.400 1.00 39.11 37.741 35.194 56.193 1.00 38.45	0
ATOM	10121 U LEUF 3/9	37.741 33.194 36.193 1.00 38.43	C
		38.318 32.362 59.508 1.00 40.15	C
ATOM	10124 CD1 LEU F 379	37 441 31 705 60 581 1.00 40.96	Č
ATOM	10125 CD2 LEU F 379	38.438 31.556 58.227 1.00 38.06	Ċ
		37.082 36.405 57.990 1.00 39.47	N
		36.254 37.307 57.205 1.00 40.79	С
		37.051 37.901 56.056 1.00 42.77	С
	10129 O GLUF 380		0
	10130 CB GLUF 380	35.715 38.422 58.054 1.00 40.39	. <b>C</b> - · ·
	10131 CG GLU F 380	34.729 37.959 59.122 1.00 43.41	C
	10132 CD GLUF 380		C
	10133 OE1 GLUF 380	35.364 40.007 60.152 1.00 47.79	0
	10134 OE2 GLU F 380	33.374 39.296 60.582 1.00 46.00	O N
	10135 N CYS F 381 10136 CA CYS F 381	38.303 38.264 56.267 1.00 44.51 39.090 38.839 55.214 1.00 45.77	C
	10130 CA C15 F 381	39.431 37.884 54.107 1.00 43.13	C
	10137 C CTS F 381	39.293 38.321 52.966 1.00 41.88	0
	10138 O C15 F 381	40.286 39.552 55.869 1.00 50.51	C
	10140 SG CYS F 381	40.155 41.305 55.384 1.00 63.88	Š
	10141 N ALA F 382	39.868 36.656 54.352 1.00 40.87	N
	10142 CA ALAF 382	40.259 35.766 53.266 1.00 39.08	С
ATOM	10143 C ALA F 382	39.347 34.668 52.779 1.00 39.12	С

wo	98/5681	2	334/371	PCT/GB98/01708
<b>ATOM</b>	10144	O ALA F 382	39.688 33.906 51.885 1.00 38.15	Ο
ATOM	10145	CB ALAF382	41.475 35.039 53.859 1.00 37.88	С
			38.133 34.521 53.295 1.00 40.06	
ATOM	10147	CA TRP F 383	37.225 33.440 52.930 1.00 38.49	С
<b>ATOM</b>	10148	C TRP F 383	37.151 33.142 51.460 1.00 38.16	С
			37.467 32.026 51.053 1.00 38.73	0
<b>ATOM</b>	10150	CB TRP F 383	35.880 33.677 53.561 1.00 38.28	С
ATOM	10151	CG TRP F 383	35.000 34.712 52.953 1.00 37.76 34.895 36.036 53.260 1.00 36.51	С
ATOM	10152	CD1 TRP F 383	34.895 36.036 53.260 1.00 36.51	С
ATOM	10153	CD2 TRP F 383	34.053 34.447 51.908 1.00 37.63	
ATOM	10154	NE1 TRP F 383	33.945 36.613 52.468 1.00 36.21	N
ATOM	10155	CE2 TRP F 383	33.420 35.675 51.625 1.00 37.28	С
ATOM	10156	CE3 TRP F 383	33.719 33.295 51.188 1.00 37.36	С
ATOM	10157	CZ2 TRP F 383	32.449 35.775 50.636 1.00 37.38	C
ATOM	10158	CZ3 TRP F 383	32.753 33.408 50.211 1.00 37.26	c
ATOM	10159	CH2 TRP F 383	32.131 34.632 49.957 1.00 37.38	C
			36.788 34.113 50.637 1.00 38.14	
			36.696 33.901 49.194 1.00 36.05	
			38.052 33.633 48.585 1.00 35.25 38.125 32.851 47.649 1.00 34.43	C O
ATOM	10163	CD LEUF 384	38.123 32.831 47.049 1.00 34.43	C
ATOM	10164	CG LEUF 384	35.928 35.038 48.559 1.00 35.43 35.605 34.008 47.078 1.00 35.80	C
			35.605 34.908 47.078 1.00 35.80 34.913 33.586 46.766 1.00 36.21	C
			34.696 36.047 46.633 1.00 35.95	
		N GLUF 385		
			40.474 33.902 48.470 1.00 36.48	C
			40.722 32.415 48.723 1.00 36.30	
ATOM	10171	O GIHE 385	41 082 31 709 47 798 1 00 36 28	
ATOM	10172	CB GLUF 385	41.621 34.721 49.025 1.00 36.55 41.919 36.044 48.377 1.00 37.81	С
ATOM	10173	CG GLU F 385	41.919 36.044 48.377 1.00 37.81	С
ATOM	10174	CD GLUF 385	42.997 36.840 49.082 1.00 40.00	С
ATOM	10175	OE1 GLU F 385	42.619 37.393 50.149 1.00 40.67	O
<b>ATOM</b>	10176	OE2 GLU F 385	44.180 36.955 48.627 1.00 40.89	Ο
ATOM	10177	N ILEF386	40.491 31.950 49.952 1.00 36.53	N
ATOM	10178	CA ILEF386	40.640 30.554 50.291 1.00 37.02	С
		C ILE F 386	39.749 29.686 49.389 1.00 37.09	С
		O ILE F 386	40.229 28.726 48.783 1.00 36.20	0
		CB ILEF386	40.250 30.145 51.708 1.00 37.27	c
		CG1 ILE F 386	40.796 31.053 52.794 1.00 39.60	C
		CG2 ILE F 386	40.758 28.731 51.927 1.00 37.45	C
		CD1 ILE F 386	42.314 31.140 52.836 1.00 40.65	C
		N LEUF 387	38.458 29.998 49.293 1.00 37.75	N
		CA LEUF 387	37.599 29.211 48.423 1.00 38.77	C
		C LEUF 387	38.125 29.170 46.978 1.00 39.37	С
ATOM	10188	O LEUF 387	38.066 28.107 46.352 1.00 40.51	О

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ATOM	10234	CD1 TRP F 393	43 801 21 410 45 415 1 00 49 59	С
ATOM	10235	CD2 TRP F 393	45,758 21,664 44,369 1.00 49.88	С
ATOM	10236	NE1 TRP F 393	45.758 21.664 44.369 1.00 49.88 44.549 20.265 45.633 1.00 50.00	N
ATOM	10237	CE2 TRP F 393	45.752 20.398 45.004 1.00 49.70	С
ATOM	10238	CE3 TRP F 393	46.888 22.060 43.645 1.00 50.21	С
		CZ2 TRP F 393		
			47.960 21.179 43.580 1.00 50.79	
ATOM	10241	CH2 TRP F 393	47.920 19.925 44.223 1.00 50.52	С
ATOM	10242	N ARG F 394	41.848 22.202 42.736 1.00 48.49	N
ATOM	10243	CA ARGF 394	41.168 20.977 42.363 1.00.48.26	С
ATOM	10244	C ARG F 394	40.768 21.048 40.897 1.00 49.54	С
<b>ATOM</b>	10245	O ARG F 394	40.361 20.055 40.307 1.00 51.77	0
ATOM	10246	CB ARGF 394	39.961 20.631 43.203 1.00 47.19	С
			38.965 21.623 43.674 1.00 45.48	
ATOM	10248	CD ARGF 394	37.928 20.983 44.585 1.00 44.46	С
ATOM	10249	NE ARG F 394	36.762 21.872 44.620 1.00 46.03	N
<b>ATOM</b>	10250	CZ ARG F 394	36.762 21.872 44.620 1.00 46.03 36.680 22.973 45.370 1.00 44.99	С
ATOM	10251	NH1 ARG F 394	37.755 23.200 46.108 1.00 44.94	N
			35.631 23.780 45.357 1.00 43.48	
			40.842 22.169 40.217 1.00 50.68	
			40.450 22.232 38.826 1.00 52.13	С
			41.637 22.045 37.903 1.00 54.26	
			41.430 22.047 36.690 1.00 54.51	
ATOM	10257	CB SER F 395	39.814 23.613 38.598 1.00 51.54	C
ATOM	10258	OG SER F 395	38.434 23.568 38.917 1.00 49.50 42.841 21.927 38.429 1.00 56.83	0
ATOM	10259	N MET F 396	42.841 21.927 38.429 1.00 56.83	N
			44.049 21.787 37.662 1.00 60.12	
			44.093 20.804 36.507 1.00 63.54	
			44.429 21.178 35.366 1.00 64.11	
			45.163 21.300 38.583 1.00 60.15	
			46.413 22.143 38.424 1.00 60.96	
		SD MET F 396	47.220 22.086 40.024 1.00 62.82	S
-		CE MET F 396	48.773 21.273 39.595 1.00 63.48 43.756 19.544 36.798 1.00 66.51	C N
-		N GLU F 397 CA GLU F 397	43.786 18.531 35.760 1.00 68.51	C
			42.540 18.502 34.931 1.00 68.28	C
		C GLU F 397 O GLU F 397	42.172 17.409 34.479 1.00 08.28	0
		CB GLUF 397	44.000 17.119 36.311 1.00 75.00	c
		CG GLUF 397	45.131 16.996 37.322 1.00 81.33	c
		CD GLUF 397	44.610 17.523 38.658 1.00 85.69	Č
		OE1 GLU F 397	43.356 17.655 38.778 1.00 87.29	Ö
		OE2 GLU F 397	45.435 17.825 39.553 1.00 88.64	Ö
_		N HIS F 398	41.743 19.522 34.719 1.00 66.05	N
		CA HIS F 398	40.551 19.495 33.880 1.00 64.49	C
		C HIS F 398	40.620 20.802 33.092 1.00 63.29	C
VI OIAI	10270	C 11101 370	10.020 20,002 33,072 1.00 03.27	<b>-</b>

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ATOM 10324 C PHE E 404	33.311 21.873 42.806 1.00 50.02	С
	33.771 21.982 43.922 1.00 50.73	ŏ
	31.990 23.733 41.802 1.00 47.90	
	32.216 25.102 41.192 1.00 48.13	
ATOM 10328 CD1 PHE F 404	32.266 25.227 39.807 1.00 47.82	
ATOM 10329 CD2 PHE F 404	32.266 25.227 39.807 1.00 47.82 32.431 26.212 41.987 1.00 47.31	C
ATOM 10330 CE1 PHE F 404	32.496 26.454 39.225 1.00 47.23	С
ATOM 10331 CE2 PHE F 404	32.680 27.437 41.405 1.00 46.93	С
ATOM 10332 CZ PHE F 404	32.702 27.548 40.037 1.00 47.49	С
	32.747 20.761 42.364 1.00 52.13	
	32.630 19.524 43.113 1.00 53.76	
ATOM 10335 C ALA F 405	33.019 18.344 42.228 1.00 54.52	; <b>C</b>
ATOM 10336 O ALA F 405	33.105 18.438 41.007 1.00 53.84	0
	31.189 19.310 43.551 1.00 53.84	
	33.143 17.180 42.867 1.00 55.35	
	33.498 15.929 42.205 1.00 55.29	
ATOM 10340 C PRO F 406		
	32.605 15.218 40.103 1.00 57.58	
	33.681 14.837 43.237 1.00 54.48	
ATOM 10343 CG PROF 406	33.704 15.630 44.504 1.00 54.71 33.007 16.957 44.301 1.00 54.88	C
	31.169 16.060 41.651 1.00 55.15	
	30.035 15.895 40.755 1.00 55.97	
	29.517 17.195 40.194 1.00 57.26	
	28.311 17.208 39.894 1.00 58.96	
	28.911 15.202 41.515 1.00 55.94	
	28.276 16.110 42.537 1.00 55.68	
	28.995 16.857 43.181 1.00 57.28	
ATOM 10352 ND2 ASN F 407	26.963 16.028 42.632 1.00 56.05	N
	30.316 18.250 40.064 1.00 57.16	N
ATOM 10354 CA LEUF 408	29,763 19.499 39.485 1.00 55.99	С
	30.968 20.067 38.746 1.00 56.37	С
	31.863 20.565 39.417 1.00 57.68	0_
ATOM 10357 CB LEUF 408	29.225 20.523 40.446 1.00 55.58	C
ATOM 10358 CG LEU F 408	28.755 21.875 39.900 1.00 55.00	С
	27.830 21.740 38.707 1.00 54.25	C
ATOM 10360 CD2 LEU F 408	27.969 22.634 40.987 1.00 54.68	C
ATOM 10361 N LEUF 409	30.970 19.890 37.442 1.00 56.60	N C
ATOM 10362 CA LEU F 409 ATOM 10363 C LEU F 409	32.144 20.327 36.665 1.00 55.96 31.710 21.289 35.590 1.00 55.95	c
ATOM 10363 C LEUF 409 ATOM 10364 O LEUF 409	31.388 20.869 34.495 1.00 57.17	0
ATOM 10304 O LEUF 409 ATOM 10365 CB LEUF 409	32.791 19.058 36.164 1.00 55.32	C
ATOM 10305 CB LEU F 409	33.947 18.979 35.213 1.00 55.70	č
	34.956 20.101 35.339 1.00 55.90	C
	34.675 17.653 35.488 1.00 56.47	Ċ

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ATOM 10260 N   FILE 410	31.667 22.577 35.902 1.00 56.56	N
ATOM 10370 CA LEUT 410	31.244 23.545 34.902 1.00 57.26	Ċ
	32.413 23.805 33.970 1.00 59.35	C
ATOM 10372 O LEUF 410	33.584 23.637 34.304 1.00 58.97	Ο
ATOM 10373 CB LEU F 410	30.668 24.837 35.464 1.00 55.77	С
ATOM 10374 CG LEU F 410	29.667 24.528 36.601 1.00 54.83	С
ATOM 10375 CD1 LEU F 410	29.205 25.798 37.278 1.00 55.52	C
ATOM 10376 CD2 LEU F 410	28.505 23.766 36.001 1.00 54.77	С
	31.952 24.202 32.790 1.00 62.19	N
ATOM 10378 CA ASP F 411	32.831 24.505 31.661 1.00 64.49	С
ATOM 10379 C ASP F 411	32.795 25.997 31.412 1.00 64.48	C
ATOM 10380 O ASP F 411	31.761 26.647 31.652 1.00 64.26	0
ATOM 10381 CB ASP F 411	32.228 23.669 30.538 1.00 68.33	C
ATOM 10382 CG ASP F 411	32.391 24.299 29.173 1.00 72.19	C
ATOM 10383 OD1 ASP F 411	31.696 25.321 28.932 1.00 73.43	0
ATOM 10384 OD2 ASP F 411	33.220 23.750 28.392 1.00 74.63	O N
	33.886 26.578 30.919 1.00 64.89	
ATOM 10386 CA ARG F 412	33.906 28.019 30.696 1.00 65.23	c
ATOM 10387 C ARGF 412	32.569 28.596 30.266 1.00 65.96 31.925 29.407 30.917 1.00 65.50	
ATOM 10388 O ARGF 412	34.982 28.444 29.689 1.00 64.44	C
ATOM 10309 CB ARG F 412	34.710 29.873 29.244 1.00 64.57	Č
ATOM 10390 CO ARG F 412	35.927 30.537 28.674 1.00 65.66	
ATOM 10392 NE ARG F 412	35.763 31.981 28.559 1.00 66.61	
ATOM 10393 CZ ARG F 412	34.857 32.600 27.815 1.00 66.99	
	33.978 31.914 27.094 1.00 66.89	
ATOM 10395 NH2 ARG F 412	34.842 33.932 27.799 1.00 67.45	N
ATOM 10396 N ASN F 413	32.083 28.198 29.112 1.00 68.07	N
	30.830 28.695 28.572 1.00 70.73	С
	29.668 28.640 29.522 1.00 70.13	C
ATOM 10399 O ASN F 413	28.805 29.535 29.411 1.00 70.65	0
ATOM 10400 CB ASN F 413	30.525 27.900 27.282 1.00 74.76	C
ATOM 10401 CG ASN F 413	31.789 28.095 26.420 1.00 78.76	С
ATOM 10402 OD1 ASN F 413	32.005 29.230 25.952 1.00 80.28	O
ATOM 10403 ND2 ASN F 413	32.560 27.007 26.279 1.00 79.96	N
ATOM 10404 N GLN F 414	29.592 27.702 30.462 1.00 68.79 28.458 27.658 31.391 1.00 68.63	C
ATOM 10405 CA GLN F 414 ATOM 10406 C GLN F 414	28.438 27.638 31.391 1.00 68.63	c
ATOM 10406 C GLN F 414  ATOM 10407 O GLN F 414	27.433 29.292 32.874 1.00 66.88	o
ATOM 10407 O GEN F 414  ATOM 10408 CB GLN F 414	28.463 26.359 32.177 1.00 69.46	C
ATOM 10408 CB GLN F 414 ATOM 10409 CG GLN F 414	28.856 25.169 31.307 1.00 70.47	Č
ATOM 10409 CG GLN F 414 ATOM 10410 CD GLN F 414	28.369 23.893 31.965 1.00 71.50	č
ATOM 10410 CB GENT 414	29.171 23.019 32.299 1.00 71.94	O
ATOM 10412 NE2 GLN F 414	27.044 23.864 32.118 1.00 72.39	N
ATOM 10413 N GLY F 415	29.596 29.527 32.400 1.00 67.80	N

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	29.746 30.770 33.128 1.00 68.11	
	28.777 31.750 32.470 1.00 68.30	
	28.072 32.412 33.224 1.00 68.90	
	28.604 31.849 31.163 1.00 69.39 27.655 32.763 30.541 1.00 70.28	
	26.246 32.690 31.106 1.00 69.50	C
	25.479 33.656 30.958 1.00 69.84	0
	27.606 32.594 29.019 1.00 71.83	C
	28.968 32.338 28.420 1.00 75.31	C
	29.289 33.295 27.285 1.00 78.73	
	29.356 32.551 25.946 1.00 81.02	
	30.705 31.935 25.732 1.00 82.82	
ATOM 10426 N CYS F 417	25.830 31.622 31.772 1.00 68.21	N
	24.503 31.540 32.358 1.00 67.61	
	24.285 32.661 33.350 1.00 65.76	
	23.207 33.256 33.316 1.00 66.11	0
	24.329 30.165 32.985 1.00 70.15	С
	24.382 28.881 31.683 1.00 77.76	S
	25.241 33.005 34.210 1.00 63.55	
ATOM 10433 CA VAL F 418	25.081 34.098 35.147 1.00 61.32	С
ATOM 10434 C VALF418	25.746 35.372 34.665 1.00 61.63	С
	26.850 35.314 34.165 1.00 61.60	0
	25.650 33.726 36.514 1.00 60.64	
	25.593 34.885 37.508 1.00 60.21	
	24.857 32.547 37.066 1.00 60.33	
	25.098 36.508 34.813 1.00 63.38	N
	25.600 37.807 34.409 1.00 65.89	
	26.960 38.096 34.988 1.00 65.05	C
	27.258 37.846 36.153 1.00 65.71	0
	24.595 38.828 34.919 1.00 70.65	C C
	24.275 39.972 33.979 1.00 77.55	C
	23.670 41.169 34.709 1.00 81.92 22.879 40.963 35.681 1.00 84.01	0
	23.980 42.334 34.320 1.00 84.04	0
ATOM 10447 OE2 GLO F 419 ATOM 10448 N GLY F 420	27.891 38.587 34.199 1.00 65.03	N
ATOM 10448 R GLY F 420	29.231 38.899 34.651 1.00 65.49	Č
ATOM 10450 C GLY F 420	30.119 37.823 35.225 1.00 64.82	c
ATOM 10451 O GLY F 420	31.218 38.147 35.713 1.00 65.72	Ö
ATOM 10452 N MET F 421	29.771 36.558 35.173 1.00 64.00	N
ATOM 10453 CA MET F 421	30.550 35.454 35.683 1.00 63.00	C
ATOM 10454 C MET F 421	31.674 34.951 34.797 1.00 61.94	C
ATOM 10455 O MET F 421	32.661 34.408 35.287 1.00 62.44	0
ATOM 10456 CB MET F 421	29.596 34.239 35.805 1.00 63.18	С
ATOM 10457 CG MET F 421	29.044 34.224 37.212 1.00 64.57	С
ATOM 10458 SD MET F 421	30.025 33.019 38.110 1.00 66.08	S

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ATOM 10459 CE MET F 421	29.018 31.565 37.788 1.00 66.03	С
ATOM 10460 N VAL F 422	31,527 35,070 33,490 1,00 60.71	N
	32.525 34.592 32.566 1.00 60.20	С
ATOM 10462 C VAL F 422	33.905 35.167 32.837 1.00 59.38	C
ATOM 10463 O VAL F 422	34.851 34.392 32.683 1.00 59.80	0
	32.263 34.966 31.088 1.00 61.22	С
	32.401 33.709 30.248 1.00 62.09	С
	30.899 35.598 30.914 1.00 62.29	C
ATOM 10467 N GLUF 423		N
	35.329 37.030 33.410 1.00 58.15	С
	35.948 36.412 34.654 1.00 55.71	C
ATOM 10470 O GLUF 423	37.152 36.166 34.665 1.00 56.58	0
ATOM 10471 CB GLUF 423	35.309 38.524 33.613 1.00 62.78	C C
ATOM 10472 CG GLUF 423	34.629 39.272 32.485 1.00 69.47	
	33.123 39.329 32.718 1.00 73.86 32.397 38.333 32.475 1.00 74.70	
	32.674 40.423 33.171 1.00 77.46	0
	35.112 36.171 35.662 1.00 51.62	N
	35.616 35.542 36.876 1.00 48.04	C
	36.031 34.137 36.507 1.00 47.89	
ATOM 10478 C ILEF 424	37.163 33.731 36.816 1.00 49.20	Ö
ATOM 10479 O ILET 424	34.548 35.642 37.941 1.00 47.10	C
	34.390 37.143 38.225 1.00 46.33	C
	34.879 34.872 39.201 1.00 46.61	C
ATOM 10483 CD1 ILE F 424	33.229 37.383 39.174 1.00 47.46	Č
	35.222 33.408 35.755 1.00 46.83	N
	35.619 32.071 35.322 1.00 48.22	С
	36.937 32.135 34.556 1.00 49.91	С
	37.853 31.316 34.702 1.00 51.00	0
ATOM 10488 CB PHE F 425	34.539 31.451 34.440 1.00 48.12	C
ATOM 10489 CG PHE F 425	33.475 30.702 35.185 1.00 49.40	С
ATOM 10490 CD1 PHE F 425	33.123 31.077 36.486 1.00 50.06	C
ATOM 10491 CD2 PHE F 425		С
ATOM 10492 CE1 PHE F 425		С
ATOM 10493 CE2 PHE F 425	31.845 28.954 35.331 1.00 50.18	С
ATOM 10494 CZ PHE F 425	31.508 29.334 36.631 1.00 50.15	С
ATOM 10495 N ASP F 426	37.069 33.148 33.702 1.00 50.26	N
ATOM 10496 CA ASP F 426	38.270 33.298 32.906 1.00 50.96	C
ATOM 10497 C ASP F 426	39.485 33.438 33.783 1.00 50.47	C
ATOM 10498 O ASP F 426	40.446 32.667 33.607 1.00 51.65	0
ATOM 10499 CB ASP F 426		С
ATOM 10500 CG ASP F 426		С
ATOM 10501 OD1 ASP F 426	37.484 32.592 30.431 1.00 58.15	0
ATOM 10502 OD2 ASP F 426		0
ATOM 10503 N MET F 427	39.441 34.345 34.750 1.00 48.52	N

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ATOM	10504	CA MET F 427	40.586 34.508 35.657 1.00 46.90	С
			40.857 33.207 36.403 1.00 45.52	
			41.990 32.747 36.614 1.00 44.26	
<b>ATOM</b>	10507	CB MET F 427	40.243 35.659 36.593 1.00 47.63	С
<b>ATOM</b>	10508	CG MET F 427	40.163 36.986 35.836 1.00 48.76	С
ATOM	10509	SD MET F 427	39.866 38.355 36.971 1.00 51.55	S
			38.139 38.222 37.326 1.00 49.51	
			39.755 32.543 36.808 1.00 43.33	
			39.933 31.284 37.518 1.00 42.21	
			40.679 30.313 36.628 1.00 43.27	
			41.685 29.742 37.071 1.00 44.04	
ATOM	10515	CG LEUF 428	38.603 30.737 37.999 1.00 40.78 38.010 31.542 39.159 1.00 40.48	C C
ATOM	10510	CD1 I FI I F 428	36.570 31.132 39.363 1.00 40.58	C
			38.790 31.334 40.446 1.00 40.90	
		N LEU F 429		
			40.881 29.212 34.467 1.00 41.90	_
			42.337 29.526 34.262 1.00 42.47	
ATOM	10522	O LEU F 429	43.205 28.654 34.401 1.00 44.16	0
ATOM	10523	CB LEU F 429	40.094 29.096 33.184 1.00 41.71 38.733 28.397 33.360 1.00 43.05	С
ATOM	10524	CG LEUF 429	38.733 28.397 33.360 1.00 43.05	С
			37.812 28.671 32.178 1.00 43.57	
			38.859 26.908 33.606 1.00 42.12	
			42.669 30.773 33.988 1.00 42.24	
			44.058 31.159 33.815 1.00 42.75 44.897 30.803 35.037 1.00 45.07	C C
			46.075 30.391 34.916 1.00 46.71	
			44.065 32.663 33.669 1.00 43.28	
ATOM	10532	N THR F 431	44.355 30.955 36.258 1.00 44.77	N
ATOM	10533	CA THR F 431	44.355 30.955 36.258 1.00 44.77 45.170 30.623 37.427 1.00 44.31	C
			45.397 29.124 37.461 1.00 44.45	С
			46.471 28.610 37.767 1.00 44.16	O
			44.451 30.999 38.735 1.00 44.07	С
			43.999 32.353 38.616 1.00 43.94	0
			45.396 30.809 39.903 1.00 43.20	C
		N SER F 432	44.289 28.452 37.131 1.00 45.50	N
		CA SER F 432 C SER F 432	44.289 26.983 37.159 1.00 47.34	C
			45.353 26.431 36.223 1.00 47.54 46.118 25.497 36.477 1.00 46.82	C O
			42.903 26.432 36.839 1.00 47.98	C
			43.039 25.012 36.825 1.00 49.24	Ö
		N SER F 433		N
			46.357 26.804 34.038 1.00 50.63	C
			47.786 27.084 34.459 1.00 51.26	С
ATOM	10548	O SER F 433	48.760 26.362 34.273 1.00 50.75	0

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ATOM 10594 C MET F 438	54.323 23.791 37.986 1.00 62.79	С
	55.142 23.592 38.867 1.00 61 09	
ATOM 10596 CB MET F 438	53.990 26.137 38.332 1.00 64.74	C
ATOM 10597 CG MET F 438	53.990 26.137 38.332 1.00 64.74 53.772 27.547 37.812 1.00 64.81	С
ATOM 10598 SD MET F 438	54.135 28.703 39.127 1.00 67.15	S
	55.311 27.925 40.183 1.00 66.27	
	53.346 22.974 37.644 1.00 63.21	
	53.225 21.673 38.262 1.00 64.74	
	53.320 21.799 39.773 1.00 63.07	
ATOM 10603 O ASN F 439	54.190 21.319 40.489 1.00 62.09	0
ATOM 10604 CB ASN F 439	54.353 20.818 37.695 1.00 69.48 54.162 19.398 38.206 1.00 73.82	C C
ATOM 10605 OD1 ASN F 439	55.154 18.664 38.273 1.00 76.98	
	52.924 19.053 38.568 1.00 75.36	
ATOM 10607 ND2 ASN 1-439 ATOM 10608 N LEU F 440		
	52.194 22.815 41.694 1.00 59.97	C
	51.887 21.539 42.469 1.00 60.37	
	50.964 20.775 42.194 1.00 60.25	
ATOM 10612 CB LEUF 440	51.075 23.839 41.882 1.00 58.78	C
ATOM 10613 CG LEUF 440	51.075 23.839 41.882 1.00 58.78 50.694 24.208 43.313 1.00 57.87	С
	51.794 25.026 43.970 1.00 56.53	С
ATOM 10615 CD2 LEU F 440	49.366 24.945 43.317 1.00 57.72	С
ATOM 10616 N GLN F 441	52.708 21.324 43.477 1.00 60.52	N
	52.558 20.194 44.348 1.00 61.60	
	51.530 20.432 45.431 1.00 61.09	
	51.343 21.567 45.857 1.00 62.04	
ATOM 10620 CB GLN F 441	53.920 20.060 45.068 1.00 64.19	С
ATOM 10621 CG GLN F 441	55.044 19.592 44.172 1.00 67.64	C
	54.612 18.553 43.142 1.00 69.80 54.443 17.386 43.525 1.00 71.77	
	54.418 18.950 41.885 1.00 69.81	
ATOM 10625 N GLY F 442	50.917 19.379 45.953 1.00 60.60	N
ATOM 10626 CA GLY F 442	49,963 19.503 47.043 1.00 58.41	C
ATOM 10627 C GLY F 442	50.664 20.048 48.283 1.00 57.04	c
ATOM 10628 O GLY F 442	50.017 20.830 48.990 1.00 57.25	O
ATOM 10629 N GLU F 443	51.920 19.742 48.570 1.00 55.94	N
ATOM 10630 CA GLU F 443	52.532 20.303 49.768 1.00 58.15	С
ATOM 10631 C GLU F 443	52.645 21.826 49.592 1.00 56.01	С
ATOM 10632 O GLU F 443	52.528 22.584 50.556 1.00 55.68	0
ATOM 10633 CB GLU F 443	53.896 19.797 50.198 1.00 62.35	C
	54.179 18.318 50.317 1.00 66.50	C
	53.709 17.564 49.077 1.00 69.75	C
	53.997 17.966 47.916 1.00 70.12	0
	52.996 16.549 49.342 1.00 72.24	O
A1UM 10038 N GLUF 444	52.894 22.219 48.348 1.00 53.52	N

ATOM	10639	CA GLUF 444	52.988 23.648 48.033 1.00 51.41	С
			51.610 24.283 48.190 1.00 49.54	С
			51.443 25.304 48.870 1.00 49.51	Ο
			53.481 23.811 46.604 1.00 51.00	С
			54.985 23.559 46.525 1.00 50.83	С
			55.461 23.611 45.082 1.00 50.64	С
			54.717 23.092 44.219 1.00 50.76	0
			56.559 24.173 44.898 1.00 49.61	O
			50.623 23.617 47.583 1.00 46.95	N
		CA PHE F 445		С
			48.842 24.458 49.124 1.00 47.00	С
			48.378 25.546 49.478 1.00 47.60	0
			48.288 23.052 47.176 1.00 43.41	С
			46.861 23.372 47.452 1.00 42.77	С
			46.282 24.521 46.973 1.00 43.64	С
			46.091 22.512 48.186 1.00 43.76	С
ATOM	10655	CELPHE F 445	44.951 24.813 47.212 1.00 44.82	С
ATOM	10656	CE2 PHE F 445	44.748 22.772 48.458 1.00 44.81	С
			44.179 23.932 47.962 1.00 45.27	С
			49.023 23.507 50.012 1.00 46.82	N
			48.660 23.616 51.425 1.00 46.58	С
			49.366 24.778 52.074 1.00 47.18	С
			48.814 25.462 52.965 1.00 47.41	0
ATOM	10662	CB VALF 446	48.850 22.180 51.966 1.00 46.32	C
			49.788 21.987 53.122 1.00 45.59	С
<b>ATOM</b>	10664	CG2 VAL F 446	47.474 21.582 52.273 1.00 46.15	С
<b>ATOM</b>	10665	N CYS F 447	50.600 25.080 51.675 1.00 46.65	N
<b>ATOM</b>	10666	CA CYS F 447	51.297 26.197 52.302 1.00 48.27	С
<b>ATOM</b>	10667	C CYS F 447	50.776 27.548 51.838 1.00 49.24	C
			50.649 28.497 52.611 1.00 49.40	О
			52.764 26.117 51.886 1.00 50.10	С
			53.656 24.982 52.943 1.00 53.85	S
			50.490 27.658 50.525 1.00 48.80	
		CA LEUF 448	49.967 28.898 49.961 1.00 46.96	C
		C LEU F 448	48.634 29.240 50.623 1.00 46.33	C
		O LEUF 448	48.356 30.354 51.071 1.00 47.24	O
		CB LEUF 448	49.753 28.756 48.470 1.00 46.50	C
		CG LEUF 448	50.982 28.820 47.584 1.00 46.81	C
		CD1 LEU F 448	50.525 28.569 46.148 1.00 48.16	C
		CD2 LEU F 448	51.731 30.124 47.684 1.00 45.78	C
		N LYS F 449	47.782 28.221 50.726 1.00 44.50	N
		CA LYS F 449	46.492 28.407 51.367 1.00 43.31	С
		C LYS F 449	46.691 28.978 52.754 1.00 42.85	C
		O LYS F 449	45.996 29.937 53.119 1.00 43.25	0
ATOM	10683	CB LYSF 449	45.749 27.103 51.327 1.00 43.90	С

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			44.247 27.263 51.191 1.00 44.78	С
ATOM	10685	CD LYS F 449	43.613 26.159 51.990 1.00 47.21	Ċ
ATOM	10686	CE LYS F 449	43.433 24.850 51.206 1.00 47.74	Č
ATOM	10687	NZ LYS F 449	42.589 24.020 52.170 1.00 50.18	N
			47.639 28.500 53.553 1.00 42.46	
			47.814 29.119 54.875 1.00 42.90	
			48.383 30.521 54.786 1.00 42.09	С
			48.029 31.365 55.595 1.00 43.54	0
ATOM	10692	CB SER F 450	48.795 28.347 55.761 1.00 43.59	С
ATOM	10693	OG SER F 450	48.248 27.029 55.787 1.00 47.77	0
ATOM	10694	N ILE F 451	49.269 30.781 53.834 1.00 40.12	N
<b>ATOM</b>	10695	CA ILE F 451	49.820 32.118 53.722 1.00 39.28	С
<b>ATOM</b>	10696	C ILE F 451	48.634 33.042 53.469 1.00 39.77	С
<b>ATOM</b>	10697	O ILE F 451	48.634 33.042 53.469 1.00 39.77 48.568 34.114 54.089 1.00 39.70	0
ATOM	10698	CB ILE F 451	50.814 32.179 52.553 1.00 40.03	<b>C</b> .
			52.019 31.314 52.972 1.00 40.96	
ATOM	10700	CG2 ILE F 451	51.168 33.605 52.181 1.00 37.43	С
ATOM	10701	CD1 ILE F 451	53.226 31.501 52.067 1.00 42.25	С
			47.705 32.616 52.586 1.00 38.84	N
			46.548 33.463 52.283 1.00 37.28	C
ATOM	10704	C ILE F 452	45.768 33.774 53.550 1.00 38.23	
ATOM	10705	O ILE F 452	45.435 34.904 53.888 1.00 38.53 45.621 32.826 51.235 1.00 35.26	0
				C
			46.372 32.603 49.939 1.00 34.97	C
ATOM	10708	CG2 ILE F 452	44.378 33.683 51.037 1.00 34.63	C
ATOM	10709	CDI ILE F 452	45.603 32.333 48.672 1.00 34.25 45.448 32.766 54.353 1.00 39.02	C N
ATOM	10710	N LEUF 453	45.448 32,760 54,353 1.00 39.02	C
			44.689 32.962 55.568 1.00 38.90 45.422 33.935 56.465 1.00 40.48	
			44.764 34.756 57.094 1.00 41.71	
ATOM	10713	CR IFILE 453	44.488 31.644 56.342 1.00 37.90	C
			43.878 31.797 57.744 1.00 35.70	
			42.461 32.331 57.605 1.00 34.11	C
		CD2 LEU F 453		Č
		N LEU F 454	46.738 33.818 56.596 1.00 41.92	N
		CA LEUF 454		C
		C LEUF 454	47.851 36.042 56.967 1.00 45.28	C
		O LEU F 454		O
		CB LEUF 454		C
		CG LEUF 454	48.483 32.896 58.962 1.00 43.99	С
		CD1 LEU F 454	49.669 31.956 58.989 1.00 44.83	С
		CD2 LEU F 454		С
ATOM	10726	N ASN F 455	48.106 36.198 55.670 1.00 46.34	N
ATOM	10727	CA ASN F 455	48.575 37.509 55.222 1.00 46.38	С
ATOM	10728	C ASN F 455	47.492 38.408 54.733 1.00 48.11	С

43.373 45.094 60.454 1.00 92.52

42.202 44.767 60.650 1.00 93.45

42.728 45.356 58.062 1.00 91.17

43.188 44.550 56.977 1.00 91.48

42.249 46.666 57.454 1.00 92.09

44.326 44.983 61.375 1.00 94.30

43.071 45.149 63.600 1.00 97.02

42.202 44.463 64.198 1.00 98.67

44.007 44.400 62.671 1.00 95.51

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ATOM 10765 C THR F 460

ATOM 10766 O THR F 460

ATOM 10767 CB THR F 460

ATOM 10768 OG1 THR F 460

ATOM 10769 CG2 THR F 460

ATOM 10770 N PHE F 461

ATOM 10771 CA PHE F 461

ATOM 10772 C PHE F 461

ATOM 10773 O PHE F 461

ATOM	10774	CB PHE F 461	45.304 43.939 63.383 1.00 94.47	С
<b>ATOM</b>	10775	CG PHE F 461	45.403 42.449 63.144 1.00 93.47	С
<b>ATOM</b>	10776	CD1 PHE F 461	44.247 41.711 62.949 1.00 93.23	С
<b>ATOM</b>	10777	CD2 PHE F 461	46.612 41.809 63.106 1.00 93.27	С
<b>ATOM</b>	10778	CE1 PHE F 461	44.292 40.364 62.725 1.00 93.64	С
<b>ATOM</b>	10779	CE2 PHE F 461	46.665 40.453 62.887 1.00 93.44	С
ATOM	10780	CZ PHE F 461	45.511 39.723 62.698 1.00 93.70	С
<b>ATOM</b>	10781	N THR F 465	46.080 48.070 69.919 1.00128.09	N
<b>ATOM</b>	10782	CA THR F 465	47.275 48.516 69.200 1.00127.92	С
<b>ATOM</b>	10783	C THR F 465	48.509 47.732 69.610 1.00126.82	C
<b>ATOM</b>	10784	O THR F 465	48.993 46.885 68.848 1.00127.12	0
<b>ATOM</b>	10785	CB THR F 465	47.529 50.024 69.364 1.00128.71	С
<b>ATOM</b>	10786	OG1 THR F 465	48.921 50.323 69.170 1.00129.08	O
<b>ATOM</b>	10787	CG2 THR F 465	47.131 50.503 70.758 1.00129.15	С
ATOM	10788	N LEU F 466	49.036 47.920 70.818 1.00124.77	N
<b>ATOM</b>	10789	CA LEUF 466	50.204 47.163 71.281 1.00122.08	С
<b>ATOM</b>	10790	C LEUF 466	49.970 45.655 71.184 1.00119.75	С
<b>ATOM</b>	10791	O LEU F 466	50.911 44.895 70.921 1.00119.76	0
<b>ATOM</b>	10792	CB LEUF 466	50.594 47.589 72.695 1.00122.35	С
<b>ATOM</b>	10796	N LYS F 467	48.732 45.190 71.374 1.00116.39	N
<b>ATOM</b>	10797	CA LYS F 467	48.391 43.782 71.229 1.00112.94	С
ATOM	10798	C LYS F 467	48.402 43.519 69.715 1.00108.91	С
ATOM	10799	O LYS F 467	48.770 42.432 69.289 1.00108.66	0
ATOM	10800	CB LYSF 467	47.052 43.372 71.822 1.00114.52	С
<b>ATOM</b>	10801	CG LYS F 467	46.877 41.889 72.158 1.00115.32	С
ATOM	10802	CD LYS F 467	45.416 41.575 72.420 1.00116.50	С
ATOM	10803	CE LYS F 467	44.993 41.530 73.881 1.00117.04	С
			43.512 41.412 74.043 1.00116.88	N
		N SER F 468		N
			48.049 44.395 67.468 1.00 99.80	С
		C SER F 468		С
			49.770 43.524 66.011 1.00 96.17	0
			47.436 45.617 66.780 1.00100.03	С
		OG SER F 468	46.057 45.693 67.060 1.00101.11	О
		N LEUF 469	50.372 45.063 67.533 1.00 92.49	N
		CA LEUF 469	51.774 45.046 67.131 1.00 88.39	С
		C LEUF 469	52.313 43.664 67.458 1.00 86.07	C
		O LEU F 469	53.102 43.098 66.707 1.00 85.58	0
		CB LEUF 469	52.515 46.211 67.760 1.00 88.53	С
		N GLU F 470	51.876 43.075 68.560 1.00 83.98	N
		CA GLUF 470	52.310 41.730 68.934 1.00 82.73	С
		C GLU F 470	51.629 40.703 68.049 1.00 78.47	C
	-	O GLU F 470	52.219 39.715 67.627 1.00 77.03	0
		CB GLUF 470	52.114 41.561 70.419 1.00 87.19	C
ATOM	10824	CG GLUF 470	51.441 40.290 70.885 1.00 93.23	С

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66.729 28.153 41.447 1.00 68.46

65.380 27.771 41.038 1.00 67.58

N

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ATOM 11052 N GLN F 499

ATOM 11053 CA GLN F 499

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ATOM 11054	C GLN F 499	64.432 27.889 42.225 1.00 66.81	С
ATOM 11055	O GLN F 499	63.232 28.169 42.074 1.00 67.73	Ο
ATOM 11056	CB GLN F 499	65.319 26.328 40.569 1.00 68.41	С
ATOM 11057	CG GLN F 499	66.569 25.956 39.797 1.00 69.77	С
ATOM 11058	CD GLN F 499	66.310 24.694 38.995 1.00 71.11	С
ATOM 11059	OE1 GLN F 499	66.251 23.602 39.570 1.00 72.06	0
ATOM 11060	NE2 GLN F 499	66.161 24.911 37.692 1.00 71.62	N
	N GLNF 500	65.002 27.639 43.405 1.00 64.28	N
ATOM 11062	CA GLN F 500	64.214 27.745 44.626 1.00 61.77	С
ATOM 11063	C GLN F 500	63.712 29.189 44.755 1.00 59.30	С
ATOM 11064	O GLN F 500	62.486 29.340 44.816 1.00 58.46	0
ATOM 11065	CB GLN F 500	65.049 27.385 45.832 1.00 62.64	С
ATOM 11066	CG GLN F 500	65.107 25.907 46.181 1.00 64.31	С
ATOM 11067	CD GLN F 500	66.332 25.698 47.072 1.00 65.36	С
ATOM 11068	OE1 GLN F 500	66.529 26.331 48.105 1.00 64.72	O
ATOM 11069	NE2 GLN F 500	67.187 24.783 46.622 1.00 66.80	N
ATOM 11070	N HISF 501	64.620 30.184 44.744 1.00 55.48	N
ATOM 11071	CA HISF 501	64.119 31.542 44.871 1.00 53.41	С
ATOM 11072	C HIS F 501	63.185 31.939 43.734 1.00 53.11	C
ATOM 11073	O HIS F 501	62.247 32.725 43.949 1.00 52.75	0
ATOM 11074	CB HIS F 501	65.178 32.569 45.105 1.00 53.16	C
ATOM 11075	CG AHIS F 501	66.179 32.918 44.074 0.50 53.76	C
ATOM 11076	CG BHIS F 501	66.317 32.267 46.012 0.50 53.33	C
ATOM 11077	ND1AHIS F 501	67.522 33.081 44.383 0.50 54.09	N
ATOM 11078	ND1BHIS F 501	66.152 31.677 47.244 0.50 53.82	N C
ATOM 11079	CD2AHIS F 501	66.066 33.154 42.746 0.50 53.48 67.651 32.485 45.885 0.50 53.10	C
ATOM 11080	CD2BHIS F 501	67.651 32.485 45.885 0.50 53.10	C
ATOM 11081	CE1AHIS F 501	68.181 33.392 43.282 0.50 54.13	C
ATOM 11082	CEIBHIS F 501	67.323 31.536 47.834 0.50 53.60	N
ATOM 11083	NEZAHIS F 501	67.317 33.439 42.276 0.50 53.75 68.248 32.021 47.025 0.50 53.22	N N
ATOM 11084	NEZBHIS F 501	63.378 31.436 42.522 1.00 52.18	N
	N GLNF 502	62.484 31.816 41.435 1.00 52.32	C
	CA GLN F 502	61.100 31.233 41.678 1.00 52.12	c
	C GLN F 502 O GLN F 502	60.091 31.951 41.667 1.00 52.45	ŏ
	CB GLN F 502	63.113 31.420 40.109 1.00 53.34	C
	CG GLN F 502	64.486 32.061 39.941 1.00 54.80	Ċ
	CD GLN F 502	65.024 32.032 38.524 1.00 55.67	Č
	OE1 GLN F 502		0
	NE2 GLN F 502		N
	N ARG F 503	60.984 29.933 41.957 1.00 50.60	N
	CA ARG F 503	59.688 29.332 42.212 1.00 48.59	C
	C ARG F 503	58.954 30.015 43.364 1.00 48.70	С
	O ARG F 503	57.745 30.238 43.219 1.00 50.52	0
	CB ARGF 503	59.831 27.858 42.594 1.00 47.57	С

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ATOM 11000 CG AR	GF 503 58 495 27 133	42.397 1.00 45.41 C
ATOM 11100 CD AR	GF 503 58.495 27.133 GF 503 58.727 25.650	42.393 1.00 43.73 C
ATOM 11101 NE AR	GF 503 57.480 24.950	42.621 1.00 44.49 N
	GF 503 56.705 24.525	
	RG F 503 57.071 24.773	
ATOM 11104 NH2 A		41.894 1.00 45.98 N
ATOM 11105 N LEU		14.458 1.00 46.15 N
	UF 504 59.049 30.989	45.576 1.00 44.20 C
ATOM 11107 C LEU		5.036 1.00 45.60 C
	JF 504 57.154 32.391 4	5.194 1.00 47.19 O
	UF 504 60.068 31.417	
ATOM 11110 CG LE	UF 504 59.490 32.000	47.927 1.00 42.00 C
ATOM 11111 CD1 LE	EU F 504 58.583 31.040	48.666 1.00 39.85 C
	EU F 504 60.603 32.448	
	A F 505 59.150 33.112 4	
	A F 505 58.598 34.338	
	AF 505 57.491 33.979 4	
	A F 505 56.432 34.596 4	
	A F 505 59.666 35.155	
	NF 506 57.605 33.000 4	
	NF 506 56.482 32.715	
	NF 506 55.251 32.319 4	
	NF 506 54.155 32.773 4	
	N F 506 56.782 31.736 LN F 506 58.224 31.567	
	LN F 506 57.742 32.436	
ATOM 11124 CO BO	LN F 506 58.566 30.641	
	LNF 506 57.033 33.378	
	LN F 506 58.054 29.525	
ATOM 11128 OFIRG	LN F 506 55.801 33.484	38.055 0.50 52.29 O
ATOM 11129 NE2AG		9 37.578 0.50 51.61 N
ATOM 11130 NE2BG		37.197 0.50 49.76 N
ATOM 11131 N LEU		2.949 1.00 46.38 N
ATOM 11132 CA LE		43.715 1.00 46.66 C
ATOM 11133 C LEU		4.417 1.00 45.94 C
ATOM 11134 O LEU	JF 507 52.323 32.487 4	4.287 1.00 46.84 O
ATOM 11135 CB LE	UF 507 54.587 30.038	44.704 1.00 48.62 C
ATOM 11136 CG LE		44.112 1.00 49.01 C
ATOM 11137 CD1 LE		45.256 1.00 49.24 C
ATOM 11138 CD2 LE		43.203 1.00 49.01 C
ATOM 11139 N LEU		5.149 1.00 44.54 N
ATOM 11140 CA LE		45.829 1.00 43.27 C
ATOM 11141 C LEU		4.860 1.00 42.96 C
ATOM 11142 O LEU		5.207 1.00 44.75 O
ATOM 11143 CB LE	UF 508 54.863 34.851	46.719 1.00 43.15 C

49.323 38.294 38.633 0.50 39.56

C

ATOM 11188 CE1AHIS F 513

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ATOM 1	1234	OG SER F 518	38.735 37.915 47.496 1.00 45.68	Ο
			38.420 40.048 44.953 1.00 43.38	N
			37,845 41.374 45.035 1.00 44.02	С
			36.755 41.433 43.982 1.00 45.82	С
ATOM I	1238	O ASN F 519	35.631 41.827 44.316 1.00 48.17	0
			38.851 42.484 44.829 1.00 45.86	C
			39.688 42.773 46.055 1.00 48.53	С
			39.121 42.742 47.157 1.00 51.16	0
ATOM 1	1242	ND2 ASN F 519	40.990 43.040 45.963 1.00 48.02	N
		N LYS F 520		N
ATOM 1	1244	CA LYS F 520	35.904 41.013 41.761 1.00 45.83	С
ATOM I	1245	C LYS F 520	34.810 40.060 42.192 1.00 45.71	С
ATOM 1	1246	O LYS F 520	33.639 40.387 42.035 1.00 47.06	0
ATOM 1	1247	CB LYS F 520	36.431 40.565 40.408 1.00 47.55	С
ATOM 1	1248	CG LYS F 520	37.777 41.261 40.186 1.00 50.89	С
			37.550 42.478 39.309 1.00 53.95	
ATOM 1	1250	CE LYS F 520	37.920 43.797 39.979 1.00 55.93	С
ATOM 1	1251	NZ LYS F 520	37.231 44.935 39.276 1.00 57.57	N
ATOM 1	1252	N GLY F 521	35.187 38.902 42.725 1.00 44.69	N
			34.155 37.980 43.169 1.00 45.45	C
		C GLY F 521		С
		O GLY F 521	32.026 38.349 44.012 1.00 45.23	0
		N MET F 522	33.685 39.299 45.278 1.00 45.57	N
			32.694 39.798 46.202 1.00 47.31	С
		C MET F 522		C
		O MET F 522		0
			33.025 40.561 47.446 1.00 47.45	C
			34.239 40.366 48.262 1.00 48.06	
			34.116 39.120 49.518 1.00 48.25	
			32.372 38.941 49.745 1.00 46.61	C
			32.444 41.697 44.684 1.00 50.85	N
		CA GLUF 523	31.683 42.716 43.982 1.00 51.12	C
		C GLUF 523	30.553 42.014 43.271 1.00 48.18	C
		O GLUF 523	29.417 42.444 43.411 1.00 49.34	0
		CB GLUF 523	32.559 43.545 43.075 1.00 57.03	C C
		CG GLUF 523 CD GLUF 523	33.168 44.774 43.713 1.00 64.59	C
		OE1 GLU F 523	32.179 45.639 44.489 1.00 69.65 30.933 45.541 44.261 1.00 72.29	0
		OE2 GLU F 523	32.644 46.455 45.342 1.00 72.29	0
		N HIS F 524	30.802 40.937 42.580 1.00 45.64	N
		CA HIS F 524	29.774 40.185 41.887 1.00 45.52	C
		C HIS F 524	28.744 39.512 42.764 1.00 45.21	c
		O HIS F 524	27.553 39.541 42.510 1.00 44.38	0
		CB HIS F 524	30.472 39.082 41.061 1.00 45.03	C
		CG HIS F 524	29.500 38.237 40.319 1.00 44.78	Č
ALOM I	1270	OO 1110 1 727	27.300 30.237 TO.317 1.00 TT.70	•

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	360/371	
	22.685 41.297 50.772 1.00 77.26	
	23.422 42.563 50.475 1.00 78.36	
ATOM 11326 N CYS F 530	21.946 41.758 45.498 1.00 75.02	N
	21.101 42.933 45.314 1.00 77.91	С
ATOM 11328 C CYS F 530		C
	18.859 42.955 44.490 1.00 80.76	0
	22.025 44.114 45.016 1.00 78.70	С
	22.899 44.546 46.566 0.50 80.09	S
	21.416 45.744 45.479 0.50 80.49	S
ATOM 11333 N LYS F 531	20.292 41.898 43.234 1.00 81.28	N
	19.308 41.500 42.243 1.00 83.47	C
ATOM 11335 C LYS F 531	18.344 40.450 42.794 1.00 84.98	C
	17.427 39.952 42.142 1.00 85.33	0
	20.012 40.877 41.037 1.00 83.89	C
	20.464 41.860 39.987 1.00 85.48	
	21.392 42.952 40.500 1.00 86.16	С
	18.525 40.011 44.022 1.00 86.63	N
	17.721 39.005 44.675 1.00 88.09	С
	17.741 37.721 43.881 1.00 86.68	C
	16.719 37.247 43.442 1.00 87.53	0
	16.298 39.519 44.872 1.00 91.72	С
	16.280 40.661 45.890 1.00 95.40	C
	16.926 40.592 46.952 1.00 96.69	0
	15.536 41.730 45.570 1.00 96.83	N
ATOM 11350 N VAL F 533	18.892 37.123 43.662 1.00 85.18	N
ATOM 11351 CA VAL F 533		C
ATOM 11352 C VAL F 533	19.706 34.836 43.834 1.00 83.84	C
	19.675 33.612 43.714 1.00 84.68	0
	20.056 36.159 41.775 1.00 83.41	C
	20.117 34.960 40.845 1.00 83.32	C C
ATOM 11356 CG2 VAL F 533	19.726 37.416 40.987 1.00 83.26	
ATOM 11357 N VAL F 334 ATOM 11358 CA VAL F 534	20.401 35.347 44.836 1.00 83.29 21.126 34.600 45.830 1.00 82.89	N C
ATOM 11358 CA VAL F 334 ATOM 11359 C VAL F 534	20.234 34.332 47.037 1.00 82.22	c
ATOM 11369 C VAL F 534 ATOM 11360 O VAL F 534	19.628 35.241 47.588 1.00 81.06	0
ATOM 11360 O VAL F 334 ATOM 11361 CB VAL F 534	22.348 35.414 46.347 1.00 83.68	C
ATOM 11361 CB VALT 334 ATOM 11362 CG1 VALT 534	23.073 34.857 47.564 1.00 83.15	C
ATOM 11362 CG1 VALT 534 ATOM 11363 CG2 VAL F 534	23.361 35.599 45.222 1.00 84.29	C
ATOM 11363 CG2 VALT 334 ATOM 11364 N PRO F 535	20.214 33.078 47.449 1.00 82.07	N
ATOM 11364 N FRO F 535	19.508 32.614 48.609 1.00 82.06	C
ATOM 11365 CA PRO F 535	20.164 33.220 49.853 1.00 82.87	c
ATOM 11366 C PROF 535 ATOM 11367 O PROF 535	21.297 33.709 49.932 1.00 82.26	0
ATOM 11367 O PRO F 535 ATOM 11368 CB PRO F 535	19.633 31.079 48.693 1.00 81.49	C
ATOM 11368 CB FRO F 535	20.394 30.730 47.465 1.00 81.39	C
ATOM 11370 CD PRO F 535	20.953 31.980 46.818 1.00 82.12	Č
111 OH 11370 CD 110 1 333	20,723 21,700 10,010 1.00 02.12	_

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ATOM	11371	N LEUF 536	19.366 33.139 50.919 1.00 84.39	N
			19.693 33.630 52.239 1.00 84.86	С
ATOM	11373	C LEUF 536	20.559 32.725 53.103 1.00 84.56	С
ATOM	11374	O LEUF 536	20.213 32.487 54.278 1.00 86.23	Ο
<b>ATOM</b>	11379	N TYR F 537	21.677 32.216 52.572 1.00 82.05	N
<b>ATOM</b>	11380	CA TYR F 537	22.533 31.381 53.423 1.00 78.76	С
<b>ATOM</b>	11381	C TYR F 537	23.201 32.364 54.386 1.00 76.46	С
<b>ATOM</b>	11382	O TYR F 537	23.824 33.347 54.003 1.00 75.39	Ο
			23.539 30.624 52.610 1.00 79.09	С
ATOM	11384	CG TYR F 537	22.933 29.696 51.593 1.00 79.66	С
<b>ATOM</b>	11385	CD1 TYR F 537	22.161 28.620 51.994 1.00 80.46	C
<b>ATOM</b>	11386	CD2 TYR F 537	23.145 29.868 50.237 1.00 80.42	C
		CE1 TYR F 537		С
			22.595 28.986 49.325 1.00 81.21	C
		CZ TYR F 537	21.829 27.923 49.737 1.00 81.37	С
		OH TYR F 537	21.273 27.056 48.831 1.00 81.44	О
			23.017 32.094 55.657 1.00 74.64	N
			23.526 32.891 56.745 1.00 72.23	С
		C ASP F 538	25.015 33.031 56.925 1.00 67.31	C
		O ASP F 538		0
			22,992 32,264 58,048 1,00 77,42	C
			21.619 32.886 58.290 1.00 82.13	C
		OD1 ASP F 538	21.513 34.116 57.981 1.00 84.34	0
		OD2 ASP F 538	20.740 32.115 58.761 1.00 84.01	0
		N LEUF 539	25.798 31.971 56.859 1.00 60.88	N
			27.242 32.127 57.052 1.00 55.96	C
		C LEUF 539		C
		O LEUF 539		0
			27.864 30.778 57.301 1.00 53.97	C
			29.311 30.610 57.718 1.00 52.16	C
			29.726 31.540 58.833 1.00 51.56	C
		CD2 LEU F 539	29.591 29.178 58.141 1.00 51.41 27.395 32.629 54.677 1.00 54.03	N
		N LEUF 540		C
		CA LEUF 540	27.856 33.296 53.469 1.00 52.36 27.484 34.776 53.536 1.00 52.20	c
		C LEU F 540 O LEU F 540	28,332 35.624 53.228 1.00 50.74	o
		CB LEUF 540	27.303 32.610 52.216 1.00 50.74	C
		CG LEU F 540	27.756 33.150 50.857 1.00 49.79	C
		CD1 LEU F 540	29.171 32.700 50.530 1.00 48.69	C
		CD1 LEU F 540	26.800 32.743 49.748 1.00 48.32	Č
		N LEUF 541	26.270 35.143 53.967 1.00 53.14	N
		CA LEUF 541	25.963 36.582 54.029 1.00 55.03	Ċ
		C LEUF 541	26.813 37.261 55.091 1.00 54.67	c
		O LEUF 541	27.143 38.445 54.954 1.00 54.78	Ö
		CB LEUF 541	24.471 36.886 54.165 1.00 57.03	C
WI OIM	11717	OD DEOLEGA	27,471 30,000 34,103 1.00 37.03	J

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ATOM 11420 CG LEUF 541	23,726 36,216 52,990 1,00 60.87	С
ATOM 11421 CD1 LEU F 541	22.211 36.325 53.131 1.00 62.44	С
ATOM 11422 CD2 LEU F 541	22.211 36.325 53.131 1.00 62.44 24.173 36.738 51.619 1.00 61.65	С
ATOM 11423 N GLUF 542	27.196 36.511 56.120 1.00 53.31	N
ATOM 11424 CA GLUF 542	28.033 37.046 57.171 1.00 52.38	С
ATOM 11425 C GLU F 542	29.400 37.380 56.588 1.00 51.98	С
ATOM 11426 O GLU F 542	29.849 38.523 56.742 1.00 52.67	0
	28.154 36.038 58.284 1.00 53.28	
ATOM 11428 CG GLU F 542	28.930 36.436 59.523 1.00 54.31	С
ATOM 11429 CD GLU F 542	28.840 35.304 60.533 1.00 55.57 27.804 34.582 60.554 1.00 56.26	С
ATOM 11430 OE1 GLU F 542	27.804 34.582 60.554 1.00 56.26	0
ATOM 11431 OE2 GLU F 542	29.816 35.135 61.288 1.00 56.01	0
ATOM 11432 N MET F 543	30.050 36.440 55.913 1.00 50.17	N
ATOM 11433 CA MET F 543	31.359 36.735 55.347 1.00 49.57	
	31.291 37.827 54.311 1.00 50.51	
	32.190 38.662 54.153 1.00 50.97	
ATOM 11436 CR MET F 543	31 904 35 443 54 756 1 00 50 18	C
ATOM 11437 CG MET F 543	31.928 34.338 55.818 1.00 50.58	С
ATOM 11438 SD MET F 543	31.928 34.338 55.818 1.00 50.58 33.300 34.608 56.968 1.00 50.53	S
ATOM 11439 CE MET F 543	32.371 34.811 58.480 1.00 51.39	С
ATOM 11440 N LEUF 544	30.213 37.872 53.532 1.00 51.70	N
ATOM 11441 CA LEUF 544	30.040 38.927 52.527 1.00 51.52	С
ATOM 11442 C LEUF 544	29.902 40.269 53.223 1.00 52.54	C
ATOM 11443 O LEUF 544	30.556 41.205 52.775 1.00 52.11	0
ATOM 11444 CB LEUF 544	28.854 38.665 51.626 1.00 50.45	С
ATOM 11445 CG LEUF 544	28.403 39.709 50.627 1.00 50.36	С
ATOM 11446 CD1 LEU F 544	28.403 39.709 50.627 1.00 50.36 29.428 40.045 49.555 1.00 49.79	С
ATOM 11447 CD2 LEU F 544	27.139 39.252 49.892 1.00 50.77	С
ATOM 11448 N ASP F 545	29.117 40.388 54.286 1.00 55.62	N
ATOM 11449 CA ASP F 545	28.960 41.663 54.963 1.00 59.04 30.246 42.176 55.552 1.00 58.92	С
ATOM 11450 C ASP F 545		
ATOM 11451 O ASP F 545	30.473 43.375 55.517 1.00 58.35	O
ATOM 11452 CB ASP F 545	27.925 41.675 56.071 1.00 63.84	С
ATOM 11453 CG ASP F 545	26.524 41.431 55.545 1.00 69.30	С
ATOM 11454 OD1 ASP F 545	26.272 41.517 54.303 1.00 71.71	О
ATOM 11455 OD2 ASP F 545	25.645 41.139 56.412 1.00 71.81	0
ATOM 11456 N ALA F 546	31.113 41.309 56.050 1.00 60.03	N
ATOM 11457 CA ALA F 546	32.383 41.737 56.626 1.00 60.35	C
ATOM 11458 C ALA F 546	33.065 42.685 55.670 1.00 61.98	С
ATOM 11459 O ALA F 546	33.609 43.684 56.084 1.00 62.84	0
ATOM 11460 CB ALA F 546	33.278 40.553 56.892 1.00 59.78	С
ATOM 11461 N HIS F 547	33.071 42.387 54.395 1.00 65.43	N
ATOM 11462 CA HIS F 547	33.678 43.150 53.341 1.00 68.65	C
ATOM 11463 C HIS F 547	33.001 44.445 53.024 1.00 73.29	C
ATOM 11464 O HIS F 547	33.676 45.455 52.845 1.00 74.87	О

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	363/371	0
ATOM 11465 CB HIS F 547	33.616 42.285 52.055 1.00 67.39	C
ATOM 11466 CG HIS F 547	34.763 41.336 52.299 1.00 66.41	C
	35.973 41.497 51.682 1.00 66.39	N C
	34.859 40.273 53.118 1.00 65.69	
ATOM 11469 CEI HIS F 547	36.787 40.556 52.092 1.00 66.04	
	36.135 39.812 52.958 1.00 65.93	N
	31.678 44.404 52.945 1.00 78.97	N
	30.955 45.658 52.630 1.00 83.75	C
ATOM 11473 C ARG F 548	31.150 46.660 53.763 1.00 84.72	C
ATOM 11474 O ARG F 548		0
	29.496 45.339 52.307 1.00 86.60	C C
	29.193 44.003 51.648 1.00 89.75	
ATOM 1147/ CD ARG F 548	29.856 43.692 50.327 1.00 92.41	C
ATOM 11478 NE ARG F 548	30.388 44.805 49.549 1.00 94.87	N
	31.341 44.762 48.623 1.00 95.85	
	31.933 43.626 48.280 1.00 96.45	
	31.701 45.895 48.025 1.00 96.58	N
TER 11482 ARG F 548	a. a.a. a.a. (a.a. ) a.a. (4	0
	31.833 28.623 45.202 1.00 35.64	
HETATM11484 C2 EST F 600		
HETATM11485 C3 EST F 600	33.867 27.496 45.667 1.00 38.21	C
HETATM11486 O3 EST F 600	34.562 26.445 46.244 1.00 40.39 34.646 28.450 44.995 1.00 37.37	0
HETATM11488 C5 EST F 600		
HETATM11489 C6 EST F 600		
HETATM11490 C7 EST F 600		C
HETATM11491 C8 EST F 600	32.749 31.882 43.516 1.00 34.38	C
HETATM11492 C9 EST F 600		
	32.552 29.616 44.525 1.00 35.41 30.593 31.193 44.697 1.00 35.14	
HETATM11494 C11 EST F 600 HETATM11495 C12 EST F 600	29.742 32.231 43.916 1.00 33.14	C
HETATM11495 C12 EST F 600 HETATM11496 C13 EST F 600	30.699 33.372 43.550 1.00 34.81	C.
HETATM11496 C13 EST F 600 HETATM11497 C14 EST F 600	31.919 32.864 42.761 1.00 33.93	Č
HETATM11498 C15 EST F 600	32.542 34.190 42.382 1.00 34.40	č
HETATM11499 C16 EST F 600	31,295 34.827 41.658 1.00 35.71	Č
HETATM11500 C17 EST F 600	30.135 34.338 42.522 1.00 35.71	Č
HETATM11500 C17 EST F 600	29.277 35.383 42.960 1.00 37.33	ŏ
HETATM11502 C18 EST F 600	31.036 34.100 44.828 1.00 34.22	č
HETATM11503 O HOHU 1	21.848 58.049 128.989 1.00 40.46	ŏ
HETATM11504 O HOHU 2	2.109 53.126 126.118 1.00 65.57	Õ
HETATM11505 O HOHU 3	6.765 53.163 127.614 1.00 50.70	0
HETATM11506 O HOHU 4	4.264 57.656 127.962 1.00 59.52	0
HETATM11507 O HOHU 5	6.775 58.196 126.015 1.00 44.53	Ö
HETATM11508 O HOHU 6	8.449 55.388 126.316 1.00 49.12	Ö
HETATM11509 O HOHU 7	18.153 50.237 127.195 1.00 54.23	Ö
THE INTERIOR OF THE PROPERTY.	10.133 30.231 121.173 1.00 37.23	_

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HETATM11510 O	HOHU 8	21.397 55.268 122.647 1.00 47.01	O
HETATM11511 O	HOHU 9		Ō
HETATM11512 O		22.790 46.040 129.344 1.00 67.31	0
HETATM11513 O	HOH U 11	11.683 46.006 112.647 1.00 59.22	0
HETATM11514 O	HOH U 12	5.895 50.660 116.043 1.00 57.86	Ο
HETATM11515 O	HOH U 13	25.458 70.001 126.746 1.00 73.20	0
HETATM11516 O	HOH U 14		0
HETATM11517 O		4.234 56.305 140.939 1.00 80.83	0
HETATM11518 O	HOHU 16		0
HETATM11519 O			0
HETATM11520 O	HOHU 18	9.168 63.071 121.769 1.00 47.72	0
HETATM11521 O		4.849 54.453 123.780 1.00 82.63	0
HETATM11522 O	HOH V 1	25.793 58.286 139.374 1.00 54.29 46.017 53.443 142.101 1.00 63.10	0
HETATM11523 O HETATM11524 O	HOH V 2 HOH V 3	40.955 53.647 140.984 1.00 43.70	0
HETATM11525 O	HOH V 4	43.837 58.030 141.000 1.00 68.06	0
HETATM11526 O	HOH V 5	40.985 58.759 142.241 1.00 56.84	0
HETATM11527 O	HOH V 6	39.196 55.915 142.293 1.00 60.34	0
HETATM11528 O	HOH V 7	29.591 50.718 141.575 1.00 61.81	Ö
HETATM11529 O	HOH V 8	26.441 55.674 145.979 1.00 50.62	Ö
HETATM11530 O	HOH V 9		Ö
HETATM11531 O	HOH V 10	25.073 46.126 139.508 1.00 71.06	O
HETATM11532 O	HOH V 11	35.174 46.176 155.833 1.00 70.58	Ö
HETATM11533 O	HOH V 12	42.188 59.305 152.020 1.00 70.34	Ο
HETATM11534 O	HOH V 13	22.227 70.293 141.263 1.00 69.38	O -
HETATM11535 O	HOH V 14	22.931 53.579 161.506 1.00 46.74	O
HETATM11536 O	<b>HOH V</b> 15	43.418 56.241 127.560 1.00 67.10	Ο
HETATM11537 O	HOH V 16	48.305 44.260 142.505 1.00 65.47	Ο
HETATM11538 O	HOH V 17	26.307 51.287 140.416 1.00 68.69	0
HETATM11539 O	HOH V 18	38.697 63.615 146.601 1.00 59.04	0
HETATM11540 O	HOH V 19	43.599 54.688 145.358 1.00 80.66	0
HETATM11541 O		18.863 40.395 92.499 1.00 45.15	0
HETATM11542 O		11.617 59.649 89.904 1.00 57.58	0
HETATM11543 O		14.408 55.490 90.256 1.00 43.01	0
HETATM11544 O		9.297 54.800 88.542 1.00 70.62	0
HETATM11545 O	HOH W 5	10.264 52.765 90.951 1.00 49.19	0
HETATM11546 O	HOH W 6	13.313 53.121 91.929 1.00 60.26	0 0
HETATM11547 O HETATM11548 O		22.771 48.299 94.041 1.00 50.96 19.297 43.390 98.603 1.00 47.61	0
HETATM11549 O		7.386 44.992 105.654 1.00 64.21	Ö
HETATM11550 O		29.628 46.851 93.188 1.00 60.24	o
HETATM11551 O		21.486 58.693 106.858 1.00 74.35	o
HETATM11552 O		6.464 54.649 100.262 1.00 68.82	ő
HETATM11553 O			Ö
HETATM11554 O	HOH W 14		O
	•	The second secon	

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HETATM11555 O	HOH W 15	13.984 53.633 76.434 1.00 70.54	0
HETATM11556 O		17.110 66.927 90.775 1.00 62.32	0
	HOH W 17	23.687 44.599 94.346 1.00 60.73	Ο
HETATM11558 O	HOH W 18	6.280 48.735 95.221 1.00 55.74	0
HETATM11559 O	HOH W 19	12.146 55.843 94.680 1.00 74.27	Ο
HETATM11560 O	HOH X 1		Ο
HETATM11561 O	HOH X 2		Ο
HETATM11562 O	HOH X 3		0
HETATM11563 O	HOH X 4	33,298 20.992 86.671 1.00 54.98	0
HETATM11564 O	HOH X 5	31.936 22.793 84.241 1.00 41.39	0
	HOH X 6	33,241 25.772 84.263 1.00 51.97	0
HETATM11566 O			0
	HOH X 8		0
	HOH X 9		0
		32.682 43.133 84.366 1.00 66.26	0
		42.892 33.559 71.691 1.00 65.92	0
		33.790 20.271 74.636 1.00 51.74	0
		12.440 31.491 79.143 1.00 57.12	0
		31.046 37.551 62.222 1.00 52.34	0
		31.421 23.945 99.377 1.00 72.53	0 0
		47.484 24.789 88.075 1.00 51.06	0
		29.439 39.000 82.982 1.00 65.46 27.652 21.245 79.034 1.00 41.31	0
		36.035 24.694 81.219 1.00 73.20	Ö
	HOH Y 1	51.022 42.856 41.650 1.00 50.42	ő
HETATM11579 O HETATM11580 O	HOH Y 2	55.305 63.132 43.048 1.00 53.02	Ö
HETATM11581 O	HOHY 3	53.204 58.251 42.745 1.00 40.49	0 .
HETATM11582 O		58.073 58.597 44.494 1.00 58.72	Ö
HETATM11583 O		57.914 56.292 42.192 1.00 47.79	ŏ
HETATM11584 O	HOH Y 6		Ö
HETATM11585 O	HOH Y 7		Ö
HETATM11586 O	•	50.324 45.115 34.825 1.00 50.83	Ö
HETATM11587 O		62.094 47.962 27.730 1.00 76.57	O
HETATM11588 O		39.885 46.806 39.557 1.00 61.46	0
HETATM11589 O		46.347 59.084 26.059 1.00 72.51	0
HETATM11590 O		61.345 58.138 33.022 1.00 56.38	0
HETATM11591 O		60.304 34.626 39.805 1.00 61.76	0
HETATM11592 O	HOH Y 14	50.352 45.472 18.863 1.00 50.26	0
HETATM11593 O	HOH Y 15	53.818 57.125 56.560 1.00 66.19	0
HETATM11594 O		48.360 68.736 42.101 1.00 67.02	0
HETATM11595 O		45.590 45.900 38.932 1.00 68.45	0
HETATM11596 O		62.449 52.794 38.213 1.00 47.80	Ο
<b>HETATM11597</b> O	HOH Y 19	55.536 59.041 38.868 1.00 68.17	Ο
HETATM11598 O	HOH Z 1	46.934 37.171 50.101 1.00 41.17	0
HETATM11599 O	HOH Z 2	34.165 20.922 47.061 1.00 50.41	0

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HETATM11600 O	HOHZ 3	36.863 25.565 47.746 1.00 48.74	0
HETATM11601 O	HOHZ 4	39.998 21.594 47.150 1.00 63.60	0
HETATM11602 O	HOHZ 5	40.839 23.368 49.585 1.00 52.11	0
HETATM11603 O	HOHZ 6	39.133 26.153 49.772 1.00 59.33	0
HETATM11604 O	HOHZ 7	38.468 36.961 50.477 1.00 47.17	0
HETATM11605 O	HOH Z 8	43.196 36.928 56.104 1.00 42.56	0
HETATM11606 O	HOHZ 9	46.400 26.653 65.467 1.00 78.67	0
HETATM11607 O	HOHZ 10	36.448 43.177 48.827 1.00 65.41	0
HETATM11608 O	HOH Z 11	28.492 31.879 62.192 1.00 59.52	0
HETATM11609 O	HOH Z 12	39.635 20.562 59.171 1.00 61.65	0
HETATM11610 O	HOHZ 13	58.948 35.086 54.821 1.00 69.60	0
HETATM11611 O	HOH Z 14	39.105 38.326 71.399 1.00 56.57	0
HETATM11612 O	HOHZ 15	41.408 24.364 34.260 1.00 75.94	0
HETATM11613 O	HOHZ 16	25.083 22.557 45.757 1.00 66.82	0
HETATM11614 O	HOH Z 17	40.578 39.812 50.158 1.00 75.22	0
HETATM11615 O	HOHZ 18	45.346 22.421 55.001 1.00 43.55	0
HETATM11616 O	HOHZ 19	37.459 24.933 52.629 1.00 75.18	0
END			

02-JUN-98

HEADER PROTEIN

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COMPND ERB RAL_TRIV_HM
REMARK 1 HOMOLOGY MODEL OF ESTROGEN RECEPTOR-BETA COMPLEXED
WITH RALOXIFENE.
REMARK 1 ONLY COORDINATES OF RESIDUES IN THE IMMEDIATE VICINITY
OF THE BINDING
REMARK 1 CAVITY WHICH DIFFER BETWEEN THE ALPHA AND BETA
ISOFORMS
REMARK 1 (I326V,L384M,M421I,F445Y) ARE INCLUDED IN THIS SET OF
COORDINATES.
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SEORES 1
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SEQRES 1 1 VAL
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            1 MET
            1 ILE
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02-JUN-98

HEADER PROTEIN

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COMPND ERB RAL TRIV HM
REMARK 1 HOMOLOGY MODEL OF ESTROGEN RECEPTOR-BETA COMPLEXED
WITH ESTRADIOL.
REMARK I ONLY COORDINATES OF RESIDUES IN THE IMMEDIATE VICINITY
OF THE BINDING
REMARK 1 CAVITY WHICH DIFFER BETWEEN THE ALPHA AND BETA
ISOFORMS
REMARK 1 (1326V,L384M,M421LF445Y) ARE INCLUDED IN THIS SET OF
COORDINATES.
REMARK 1
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SEORES 1
           1 MET
SEQRES 1
SEORES 1
           1 ILE
           1 TYR
SEQRES 1
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CONECT 59 51
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## **PCT**

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#### INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

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**A3** 

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(71) Applicant (for all designated States except US): KARO BIO AB [SE/SE]; Novum, S-141 57 Huddinge (SE).

(72) Inventors; and

(75) Inventors/Applicants (for US only): ÖHMAN, Lars [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). BONN, Tomas [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). CARLQUIST, Mats [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). ENGSTRÖM, Owe [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). GOEDE, Patrick [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). HEDFORS, Åsa [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). Holdinge (SE). Holdinge (SE). Koehler, Konrad [SE/SE]; Karo Bio AB, Novum, S-141 57 Huddinge (SE). BZOZOWSKI, Andrzeji, Marek [GB/GB]; The University

of York, Heslington, York YO1 5DD (GB). PIKE, Ashley, Charles, William [GB/GB]; The University of York, Heslington, York YO1 5DD (GB). HUBBARD, Roderick, Eliot [GB/GB]; The University of York, Heslington, York YO1 5DD (GB).

- (74) Agent: WITHERS & ROGERS; 4 Dyer's Buildings, Holborn, London EC1N 2JT (GB).
- (81) Designated States: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, ARIPO patent (GH, GM, KE, LS, MW, SD, SZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG).

#### Published

With international search report.

Before the expiration of the time limit for amending the claims and to be republished in the event of the receipt of amendments.

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(54) Title: ESTROGEN RECEPTOR CRYSTALS AND LIGANDS

#### (57) Abstract

Crystal comprising at least part of the ER $\alpha$  ligand binding domain, optionally bound to a ligand, ligands that bind to ER receptors, and methods of designing them, and a homology model of the ER $\beta$  receptor.

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Int Honel Application No PCT/GB 98/01708

A. CLASSII IPC 6	FICATION OF SUBJECT MATTER C07K14/72 C07D333/54 C07D33 C07D409/04 C07D417/04 C07J41	- · - · · · · · · · · · · · · · · · · ·	07D333/60	
According to	International Patent Classification (IPC) or to both national class	fication and IPC		
	SEARCHED			
Minimum do IPC 6	cumentation searched (classification system followed by classific CO7K CO7J	ation symbols)		
Documentat	ion searched other than minimum documentation to the extent the	at such documents are included in the fie	elds searched	
Electronic d	ata base consulted during the international search (name of data	base and, where practical, search terms	s used)	
C. DOCUME	ENTS CONSIDERED TO BE RELEVANT			
Category *	Citation of document, with indication, where appropriate, of the	relevant passages	Relevant to claim No.	
Y	ANSTEAD G M ET AL: "The estrad pharmacophore: Ligand structure receptor binding affinity relat and a model for the receptor bi STEROIDS, vol. 62, no. 3, March 1997, pag XP004057108 SAN FRANCISCO US cited in the application see page 285 - page 286 see page 287 - page 297	-estrogen ionships nding site"	1	
X Furti	her documents are listed in the continuation of box C.	Patent family members are	listed in annex.	
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	actual completion of the international search  5 December 1998	Date of mailing of the internation		
			·····	
Name and r	mailing address of the ISA  European Patent Office, P.B. 5818 Patentlaan 2  NL - 2280 HV Rijswijk  Tel. (+31-70) 340-2040, Tx. 31 651 epo nl,  Fax: (+31-70) 340-3016	Authorized officer  Rufet, J		

3

Intervious Application No PCT/GB 98/01708

	etion) DOCUMENTS CONSIDERED TO BE RELEVANT	
Category *	Citation of document, with indication where appropriate, of the relevant passages	Relevant to claim No.
X	EKENA K ET AL.: "Identification of amino acids in the hormone binding domain of the human estrogen receptor important in estrogen binding" JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 271, no. 33, 16 August 1996, pages 20053-20059, XP002075903 US see page 20056, column 2 - page 20059, column 1	13,14
X	EKENA K ET AL.: "Different residues of the human estrogen receptor are involved in the recognition of structurally diverse estrogens and antiestrogens"  JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 272, no. 8, 21 February 1997, pages 5069-5075, XP002075904  BALTIMORE US see the whole document	13,14
Y	BOURGUET W ET AL.: "Crystal structure of the ligand-binding domain of the human nuclear receptor RXR-alpha" NATURE., vol. 375, 1 July 1995, pages 377-382, XP002075905 LONDON GB	1
Α	see the whole document	6,7,52
Α	GREENE G L ET AL: "SEQUENCE AND EXPRESSION OF HUMAN ESTROGEN RECEPTOR COMPLEMENTARY DNA" SCIENCE, vol. 231, no. 4742, 7 March 1986, pages 1150-1154, XP000611679 washington us see the whole document	1-4,55
A	WO 97 09348 A (KARO BIO AB) 13 March 1997 see the whole document	1-4,7,8, 56,58
A	SEIELSTAD D A ET AL: "ANALYSIS OF THE STRUCTURAL CORE OF THE HUMAN ESTROGEN RECEPTOR LIGAND BINDING DOMAIN BY SELECTIVE PROTEOLYSIS/MASS SPECTROMETRIC ANALYSIS" BIOCHEMISTRY., vol. 34, no. 39, 1995, pages 12605-12615, XP002063749 EASTON, PA US see the whole document	1-4,7,8
	-/	

3

Inti Ional Application No
PCT/GB 98/01708

C.(Continua	ation) DOCUMENTS CONSIDERED TO BE RELEVANT	
Category <sup>3</sup>	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	DANIELIAN P S ET AL: "IDENTIFICATION OF A CONSERVED REGION REQUIRED FOR HORMONE DEPENDENTTRANSCRIPTIONAL ACTIVATION BY STEROID HORMONE RECEPTORS" EMBO JOURNAL., vol. 11, no. 3, March 1992, pages 1025-1033, XP000611428 EYNSHAM, OXFORD GB see the whole document	1-4,13, 14
A	GRESE T A ET AL.: "Structure-activity relationships of selective estrogen receptor modulators: modifications to the 2-arylbenzothiophene core of raloxifene" JOURNAL OF MEDICINAL CHEMISTRY., vol. 40, 17 January 1997, pages 146-167, XP002075906 WASHINGTON US	13,14
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C.(Continua	ation) DOCUMENTS CONSIDERED TO BE RELEVANT	
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Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)
This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:
1. X Claims Nos.: because they relate to subject matter not required to be searched by this Authority, namely:  Remark: Although claim 53 could, at least partially, be considered as a mere presentation of information (Rule 39.1(v) PCT), and claim 54 at least partially as a computer programme (Rule 39.1(vi) PCT), the search has been carried out as far as possible in our systematic documentation.  2. Claims Nos.: because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:
3. Claims Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).  Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)
This International Searching Authority found multiple inventions in this international application, as follows:
see additional sheet
As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
2. As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
4. No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:
Remark on Protest  The additional search fees were accompanied by the applicant's protest.  No protest accompanied the payment of additional search fees.

#### FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

This International Searching Authority found multiple (groups of) inventions in this international application, as follows:

1. Claims: 1-15,52-58

Crystals of ER-alpha and their use in a method for designing ligands which bind to an ER. Machine-radable storage medium capable of displaying a graphical three-dimensional representation of ER crystals. A method for evaluating the ability of a chemical to associate with an estrogen receptor employing computational means to perform a fitting operation.

2. Claims: 16-27 completely and 38,39,42,43,50,59-63 partially

Ligands for estrogen receptors. Ligands which have the general structure of formula Z. Pharmaceutical compositions containing these ligands and use thereof.

3. Claims: 28-31,37,45,51 completely and 35,36,38,39,42,43,48, 49,50,59-63 partially

As invention 2 but limited to an ER-alpha or ER-beta selective ligand, which is a 2'-,3'-,5'-,6'-substituted 2-aryl benzothiophene

4. Claims: 32-34 completely and 59-63 partially

As invention 2 but limited to an ER ligand capable of filling the hydrophobic cavity of ER-alpha

5. Claims: 35,36,48,49,59-63 partially

As invention 2 but limited to an ER-alpha or ER-beta selective ligand, which is a position 3 substituted estradiol

6. Claims: 40,41,44 completely and 42,59-63 partially

As invention 2 but limitd to an ER-beta selective ligand, which is a steroid nucleus with substitutions larger than methyl at the alpha 14, 16 or 17 positions

7. Claims: 46,47 completely and 59-63 partially

As inventon 2 but limited to an ER-alpha or ER-beta selective ligand which is a 6,3'-dihydroxybenzothiophene with substitutions larger than methyl at the R2' and/or R3' position

Information on patent family members

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